Name: Pavlo Polishchuk
Date of birth: July 29, 1979
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EDUCATION:

2009	PhD in bioorganic chemistry A.V. Bogatsky Physico-Chemical Institute of National Academy of Science of Ukraine, Odessa, Ukraine (supervisor Prof. V.E. Kuz'min)
1996-2001	Master's degree in chemistry, Odessa National University, Odessa, Ukraine

WORK EXPERIENCE:

Aug 2015 – Present	Senior researcher at Institute of Molecular and Translational Medicine, Palacky University, Olomouc, Czech Republic
Jul 2014 – Jul 2015	Senior researcher at A.V. Bogatsky Physico-Chemical Institute of National Academy of Sciences of Ukraine, Odessa, Ukraine
Mar 2011 – Dec 2012	PostDoc at Laboratory of Chemoinformatics of Strasbourg University, Strasbourg, France
July 2010 – June 2014	Scientific associate at A.V. Bogatsky Physico-Chemical Institute of National Academy of Sciences of Ukraine, Odessa, Ukraine
Nov 2004 – June 2010	Junior researcher in A.V. Bogatsky Physico-Chemical Institute of National Academy of Sciences of Ukraine, Odessa, Ukraine
Nov 2000 – Oct 2001	Engineer at A.V. Bogatsky Physico-Chemical Institute of National Academy of Sciences of Ukraine, Odessa, Ukraine

LECTURES AND WORKSHOPS:

Sept 2019	Invited speaker at the Mendeleev Congress (St.Petersburg, Russia) "Chemical library design: revising the Lipinski rule"
2017, 2018, 2019	Co-organizer and lecturer at the Advanced in silico drug design workshop/hackaton (Palacky University, Olomouc, Czech Republic). http://fch.upol.cz/en/research/conferences-workshops/4add/ (2019) http://fch.upol.cz/en/research/conferences-workshops/3add (2018) http://fch.upol.cz/en/teaching/advanced-in-silico-drug-design-add/ (2017)
July 2017	Invited speaker at the Third Kazan Summer School on Chemoinformatics (Kazan, Russia) - "Virtual screening in drug discovery"
2016-present	Lecturer "Rational drug design" (Palacky University, Olomouc, Czech Republic)
Oct 2016	Invited speaker at the Autumn School on Chemoinformatics. (Munich, Germany, BIGCHEM project) http://qsar4u.com/pages/python_tutorial.php http://qsar4u.com/pages/rdkit_tutorial.php
Sept 2016	Invited speaker at the International symposium "From empirical to predictive chemistry" within the XX Mendeleev Congress (Ekaterinburg, Russia) -"Structure-based drug design"
Dec 2014	Invited speaker at the industry workshop "In Silico ADMET prediction" (EMBL-EBI, Hinxton, UK) http://qsar4u.com/files/EBI_workshop_2014_Polishchuk.pdf
July 2014	Lectures and tutorials "Introduction to R and modeling with R" at A.V. Bogatsky Physico-Chemical Institute of National Academy of Science of Ukraine (Odessa, Ukraine): http://qsar4u.com/pages/rtutorial.php

GRANTS

2018-2020	LTARF18013 (INTER-EXCELLENCE, podprogram INTER-ACTION), Ministry of education, youth and sport "Improve the output of primary screening of biologically active compounds using computational models" (principal investigator)
2014-2018	№ 14-43-00024 of Russian Scientific Foundation "Chemoinformatics approaches to organic and metabolic reactions: from empirical to predictive chemistry" (contributor)
2016	OPEN-7-23 of IT4I supercomputer center in Ostrava "Flexible docking in drug development" (principal investigator)

MAIN RESPONSIBILITIES:

1) support of medicinal chemistry projects related to development of biologically active compounds using machine learning methods, pharmacophore modeling, molecular docking;
2) analysis of HTS data
3) revealing of structure-activity relationships, virtual screening and design of novel compounds
4) development of approaches and software for modeling and prediction of compound properties

PhD students

2016-present	Mariia Matveieva, "Automatic mining of structure-activity relationships from chemical datasets"
2019-present	Alina Kutlushina, „Development of 3D pharmacophore signatures and their application in drug design"
2019-present	Aleksandra Nikonenko, „In silico design of compounds with desired properties"

PostDocs

2018-present	Olena Mokshyna - molecular dynamic studies for drug design

Reviewer in Journal of Chemical Information and Modeling, Molecular Informatics, ChemMedChem, Computational and Structural Biotechnology Journal, Combinatorial Chemistry & High Throughput Screening, Industrial & Engineering Chemistry Research, Molecules, International Journal of Molecular Science, PLOS One.

DEVELOPED APPROACHES AND THEIR OPEN SOURCE IMPLEMENTATIONS:

Molecular representation of single compounds, mixtures, quasi-mixtures and chemical reactions to encode chemical entities for QSAR modeling studies. Open-source implementation is available at https://github.com/DrrDom/sirms

Structural and physicochemical interpretation of QSAR/QSPR models applicable to any model regardless machine learning method and descriptors used. The automated workflow of QSAR/QSPR model building, validation and interpretation with graphical user interface and the supplementary R package for analysis of fragment contributions are available at: https://github.com/DrrDom/spci and https://github.com/DrrDom/rspci

3D pharmacophore signatures/hashes/fingerprints to identify identical 3D pharmacophores - https://github.com/DrrDom/pmapper. The open-source 3D ligand-based pharmacophore modeling tool - https://github.com/meddwl/psearch. Retrieval of pharmacophores from molecular dynamic simulations and virtual screening using the novel conformer coverage approach - https://github.com/ci-lab-cz/pharmd

PUBLICATIONS:
book chapters: 5
articles in peer-reviewed journals: 54
conference papers: > 100
h-index: 13 (WOS)

Selected recent publication (2015-2019)

1. Polishchuk, P. G.; Samoylenko, G. V.; Khristova, T. M.; Krysko, O. L.; Kabanova, T. A.; Kabanov, V. M.; Kornylov, A. Y.; Klimchuk, O.; Langer, T.; Andronati, S. A.; Kuz'min, V. E.; Krysko, A. A.; Varnek, A., Design, Virtual Screening, and Synthesis of Antagonists of αIIbβ3 as Antiplatelet Agents. *Journal of Medicinal Chemistry* **2015,** 58, (19), 7681-7694.
2. Krysko, A. A.; Kornylov, A. Y.; Polishchuk, P. G.; Samoylenko, G. V.; Krysko, O. L.; Kabanova, T. A.; Kravtsov, V. C.; Kabanov, V. M.; Wicher, B.; Andronati, S. A., Synthesis, biological evaluation and molecular docking studies of 2-piperazin-1-yl-quinazolines as platelet aggregation inhibitors and ligands of integrin αIIbβ3. *Bioorganic & Medicinal Chemistry Letters* **2016,** 26, (7), 1839-1843.
3. Polishchuk, P.; Tinkov, O.; Khristova, T.; Ognichenko, L.; Kosinskaya, A.; Varnek, A.; Kuz'min, V., Structural and Physico-Chemical Interpretation (SPCI) of QSAR Models and Its Comparison with Matched Molecular Pair Analysis. *Journal of Chemical Information and Modeling* **2016,** 56, (8), 1455-1469.
4. Klimenko, K.; Lyakhov, S.; Shibinskaya, M.; Karpenko, A.; Marcou, G.; Horvath, D.; Zenkova, M.; Goncharova, E.; Amirkhanov, R.; Krysko, A.; Andronati, S.; Levandovskiy, I.; Polishchuk, P.; Kuz'min, V.; Varnek, A., Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. *Bioorganic & Medicinal Chemistry Letters* **2017,** 27, (16), 3915-3919.
5. Polishchuk, P., Interpretation of Quantitative Structure–Activity Relationship Models: Past, Present, and Future. *Journal of Chemical Information and Modeling* **2017,** 57, (11), 2618-2639.
6. Polishchuk, P.; Madzhidov, T.; Gimadiev, T.; Bodrov, A.; Nugmanov, R.; Varnek, A., Structure–reactivity modeling using mixture-based representation of chemical reactions. *J Comput Aided Mol Des* **2017,** 31, (9), 829-839.
7. Kutlushina, A.; Khakimova, A.; Madzhidov, T.; Polishchuk, P., Ligand-Based Pharmacophore Modeling Using Novel 3D Pharmacophore Signatures. *Molecules* **2018,** 23, (12), 3094.
8. Matveieva, M.; Cronin, M. T. D.; Polishchuk, P., Interpretation of QSAR Models: Mining Structural Patterns Taking into Account Molecular Context. *Molecular Informatics* **2018**.
9. Nowikow, C.; Fuerst, R.; Kauderer, M.; Dank, C.; Schmid, W.; Hajduch, M.; Rehulka, J.; Gurska, S.; Mokshyna, O.; Polishchuk, P.; Zupkó, I.; Dzubak, P.; Rinner, U., Synthesis and biological evaluation of cis-restrained carbocyclic combretastatin A-4 analogs: Influence of the ring size and saturation on cytotoxic properties. *Bioorganic & Medicinal Chemistry* **2019,** 27, (19), 115032.
10. Polishchuk, P.; Kutlushina, A.; Bashirova, D.; Mokshyna, O.; Madzhidov, T., Virtual Screening Using Pharmacophore Models Retrieved from Molecular Dynamic Simulations. *International Journal of Molecular Sciences* **2019,** 20, (23), 5834.