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EDUCATION:

2009	PhD in bioorganic chemistry "Affinity of 5-HT_{1A} receptors to their ligands. QSAR analysis with the aim of hierarchical system of models on the basis of simplex representation of molecular structure" 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

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"
2020-present	Guzel Minibaeva, „De novo design of synthetically feasible compounds"

Lectures, invited lectures on conferences and workshops:

23-26 Jan 2018 21-25 Jan 2019 3-7 Feb 2020	The co-organizer and the lecturer at the annual workshops „Advanced in silico drug design" (Palacky University, Olomouc, Czech Republic). http://fch.upol.cz/en/research/conferences-workshops/3add/ https://fch.upol.cz/en/research/conferences-workshops/4add/ https://fch.upol.cz/en/research/conferences-workshops/5add/
Sept 2019	invited speaker at the simposium "From Empirical to Predictive Chemistry" on Mendeleev Congress (St.Petersburg, Russia) - "Chemical library design: revising the Lipinski rule"
2016-2020	Lectures "Rational drug design" (Palacky University, Olomouc, Czech Republic)
Oct 2016	Invited speaker at the Autumn School on Chemoinformatics. Tutorials on Python programming and introduction to RDKit (Munich, Germany, BIGCHEM project) http://qsar4u.com/pages/python_tutorial.php http://qsar4u.com/pages/rdkit_tutorial.php
Dec 2014	Invited speaker at industry workshop "In Silico ADMET prediction" of The European Bioinformatics Institute (EMBL-EBI, Hinxton, UK) "Exploring the

	black box: structural and functional interpretation of QSAR models. (Automatic exploration of datasets using QSAR)" http://qsar4u.com/files/EBI_workshop_2014_Polishchuk.pdf
Mar 2013	Invited lecturer with the course "Computer-aided drug development: structure and ligand-based approaches" in University of Silesia (Katowice, Poland): http://qsar4u.com/pages/present.php

Grants

Jan 2018-Dec 2020	LTARF18013 (program INTER-EXCELLENCE, podprogram INTER-ACTION), Ministry of education, youth and sport "Improve the output of primary screening of biologically active compounds using computational models" (MSMT-5727/2018-2) (principal investigator)
Oct 2014 – Dec 2018	№ 14-43-00024 of Russian Scientific Foundation "Chemoinformatics approaches to organic and metabolic reactions: from empirical to predictive chemistry" (contributor)

Honors and awards

March 2021	Dean's award for significant publication activity in 2020 (Faculty of Medicine and Dentistry, Palacky University)
May 2013	Winner of innovative projects contest (Odessa innovative informational center INVAC) – "New approach of development of inhibitors of platelet aggregation which are promising cardiovascular drugs"
Nov – Dec 2012	Short-term scholarship of French Embassy in Ukraine for young scientists
Oct 2009 – Aug 2011	Scholarship for young scientists of National Academy of Sciences of Ukraine.

Guest editor

Pharmaceuticals, special issue "Pharmacophore Modeling and Applications in Drug Discovery: Challenges and Recent Advances" https://www.mdpi.com/journal/pharmaceuticals/special_issues/Pharmacophore

Reviewer in Molecular Informatics, Journal of Chemical Information and Modeling, Combinatorial Chemistry & High Throughput Screening, Industrial & Engineering Chemistry Research, Molecules, International Journal of Molecular Science, PLOS One, ChemMedChem, Neurochemistry International, ACS Omega, Journal of Medicinal Chemistry, Pharmaceuticals.

Author of chemoinformatic approaches, software and web applications:

1) open-source framework for de novo structure generation by chemically reasonable mutations **CReM** (https://github.com/DrrDom/crem, https://crem.imtm.cz)
2) open-source pharmacophore modeling tools: pharmacophore perception and manipulation – **pmapper** (https://github.com/DrrDom/pmapper), automatic ligand-based pharmacophore modeling - **psearch** (https://github.com/meddwl/psearch), MD pharmacophore modeling – **pharmd** (https://github.com/ci-lab-cz/pharmd)
3) **multi-instance learning (MIL)** approach (https://github.com/dzankov/3D-MIL-QSAR)
4) open-source software tool and web-application for **automatic knowledge mining of datasets (SPCI)**: http://qsar4u.com/pages/sirms_qsar.php, https://spci.imtm.cz
5) open-source implementation of fast algorithm of calculation of **simplex descriptors (SiRMS)**, which is available on GitHub: https://github.com/DrrDom/sirms. Multi-threaded calculation of simplex descriptors of single compounds, mixtures, quasi-mixtures and reactions.
6) CF program for developing of QSAR models based on **Random Forest** approach (single-task and multi-task learning) and their subsequent analysis and usage (interpretation of models, prediction of new datasets, etc). Full version of the program is available free of charge on http://qsar4u.com/pages/rf.html.

PUBLICATIONS:

book chapters – 5,
articles in peer-reviewed journals – 62,
conference papers – 100+.