Dmitry A Filimonov

List of Publications by Year in Descending Order

96 papers	3,942 citations	32 h-index	61 g-index
106 ext. papers	4,779 ext. citations	4.5 avg, IF	5.24 L-index

#	Paper	IF	Citations
96	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain.. *Computational Biology and Chemistry*, **2022**, 98, 107674	3.6	0
95	Machine Learning Methods in Antiviral Drug Discovery. *Topics in Medicinal Chemistry*, **2021**, 245-279	0.4	0
94	TCR-PRED WEB SERVICE FOR PREDICTING THE SPECIFICITY OF EPITOPES FOR TCR CDR3 SEQUENCES BASED ON THEIR STRUCTURAL FORMULAS **2021**, 1, 212-214	0	
93	Extraction of Data on Parent Compounds and Their Metabolites from Texts of Scientific Abstracts. *Journal of Chemical Information and Modeling*, **2021**, 61, 1683-1690	6.1	0
92	In Silico Prediction of Drug-Drug Interactions Mediated by Cytochrome P450 Isoforms. *Pharmaceutics*, **2021**, 13,	6.4	4
91	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. *Molecular Informatics*, **2021**, 40, e2000231	3.8	2
90	Data and Text Mining Help Identify Key Proteins Involved in the Molecular Mechanisms Shared by SARS-CoV-2 and HIV-1. *Molecules*, **2020**, 25,	4.8	6
89	Combined network pharmacology and virtual reverse pharmacology approaches for identification of potential targets to treat vascular dementia. *Scientific Reports*, **2020**, 10, 257	4.9	9
88	A Computational Approach for the Prediction of Treatment History and the Effectiveness or Failure of Antiretroviral Therapy. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	6
87	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
86	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. *Molecular Informatics*, **2020**, 39, e2000093	3.8	13
85	Prediction of Protein-ligand Interaction Based on Sequence Similarity and Ligand Structural Features. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
84	Computer-Aided Estimation of Biological Activity Profiles of Drug-Like Compounds Taking into Account Their Metabolism in Human Body. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
83	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. *Bioinformatics*, **2020**, 36, 978-979	7.2	5
82	Data Mining Approach for Extraction of Useful Information About Biologically Active Compounds from Publications. *Journal of Chemical Information and Modeling*, **2019**, 59, 3635-3644	6.1	8
81	Drug-drug interaction prediction using PASS. *SAR and QSAR in Environmental Research*, **2019**, 30, 655-664	3.5	8
80	Improving (Q)SAR predictions by examining bias in the selection of compounds for experimental testing. *SAR and QSAR in Environmental Research*, **2019**, 30, 759-773	3.5	1

79	PASS-based prediction of metabolites detection in biological systems. *SAR and QSAR in Environmental Research*, **2019**, 30, 751-758	3.5	4
78	Assessment of the cardiovascular adverse effects of drug-drug interactions through a combined analysis of spontaneous reports and predicted drug-target interactions. *PLoS Computational Biology*, **2019**, 15, e1006851	5	5
77	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. *Journal of Chemical Information and Modeling*, **2019**, 59, 4513-4518	6.1	9
76	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. *Current Topics in Medicinal Chemistry*, **2019**, 19, 319-336	3	12
75	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. *Molecules*, **2019**, 25,	4.8	2
74	Prediction of Protein-Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. *International Journal of Molecular Sciences*, **2019**, 21,	6.3	7
73	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. *Molecules*, **2019**, 24,	4.8	6
72	Metatox - Web application for generation of metabolic pathways and toxicity estimation. *Journal of Bioinformatics and Computational Biology*, **2019**, 17, 1940001	1	8
71	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. *Bioinformatics*, **2018**, 34, 710-712	7.2	13
70	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. *Frontiers in Chemistry*, **2018**, 6, 133	5	16
69	CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds. *PLoS ONE*, **2018**, 13, e0191838	3.7	62
68	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. *Biomedical Chemistry Research and Methods*, **2018**, 1, e00004	0.4	63
67	ADVERPred-Web Service for Prediction of Adverse Effects of Drugs. *Journal of Chemical Information and Modeling*, **2018**, 58, 8-11	6.1	34
66	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of K and IC Values of Antitarget Inhibitors. *Frontiers in Pharmacology*, **2018**, 9, 1136	5.6	9
65	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. *Molecules*, **2018**, 23,	4.8	12
64	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. *Molecular Informatics*, **2017**, 36, 1600142	3.8	9
63	Web Resources for Discovery and Development of New Medicines. *Pharmaceutical Chemistry Journal*, **2017**, 51, 91-99	0.9	15
62	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobiotics' Metabolites. *Journal of Chemical Information and Modeling*, **2017**, 57, 638-642	6.1	32

61	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. *Pharmaceutical Chemistry Journal*, **2017**, 50, 775-780	0.9	11
60	PASS-based approach to predict HIV-1 reverse transcriptase resistance. *Journal of Bioinformatics and Computational Biology*, **2017**, 15, 1650040	1	7
59	QNA-Based Prediction of Sites of Metabolism. *Molecules*, **2017**, 22,	4.8	5
58	Prediction of metabolites of epoxidation reaction in MetaTox. *SAR and QSAR in Environmental Research*, **2017**, 28, 833-842	3.5	10
57	Integral estimation of xenobiotics□toxicity with regard to their metabolism in human organism. *Pure and Applied Chemistry*, **2017**, 89, 1449-1458	2.1	7
56	Computer-aided prediction of xenobiotic metabolism in the human body. *Russian Chemical Reviews*, **2016**, 85, 854-879	6.8	17
55	Online resources for the prediction of biological activity of organic compounds. *Russian Chemical Bulletin*, **2016**, 65, 384-393	1.7	16
54	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. *Journal of Cheminformatics*, **2016**, 8, 68	8.6	19
53	Prediction of amino acid positions specific for functional groups in a protein family based on local sequence similarity. *Journal of Molecular Recognition*, **2016**, 29, 159-69	2.6	4
52	Capacities of computer evaluation of hidden potential of phytochemicals of medicinal plants of the traditional Indian Ayurvedic medicine. *Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry*, **2016**, 10, 43-54	0.4	1
51	PASS Targets: Ligand-based multi-target computational system based on a public data and naïve Bayes approach. *SAR and QSAR in Environmental Research*, **2015**, 26, 783-93	3.5	32
50	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. *Journal of Chemical Information and Modeling*, **2015**, 55, 1388-99	6.1	26
49	Identification of drug targets related to the induction of ventricular tachyarrhythmia through a systems chemical biology approach. *Toxicological Sciences*, **2015**, 145, 321-36	4.4	8
48	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. *Bioinformatics*, **2015**, 31, 2046-8	7.2	55
47	Metabolism site prediction based on xenobiotic structural formulas and PASS prediction algorithm. *Journal of Chemical Information and Modeling*, **2014**, 54, 498-507	6.1	42
46	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. *Chemistry of Heterocyclic Compounds*, **2014**, 50, 444-457	1.4	340
45	Identification of drug-induced myocardial infarction-related protein targets through the prediction of drug-target interactions and analysis of biological processes. *Chemical Research in Toxicology*, **2014**, 27, 1263-81	4	11
44	Design, synthesis and pharmacological evaluation of novel vanadium-containing complexes as antidiabetic agents. *PLoS ONE*, **2014**, 9, e100386	3.7	16

43	DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula. *Bioinformatics*, **2013**, 29, 2062-3	7.2	55
42	Virtual Screening for Potential Substances for the Prophylaxis of HIV Infection in Libraries of Commercially Available Organic Compounds. *Pharmaceutical Chemistry Journal*, **2013**, 47, 343-360	0.9	3
41	Fragment-based design, docking, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors. *European Journal of Medicinal Chemistry*, **2012**, 47, 111-24	6.8	61
40	Quantitative prediction of antitarget interaction profiles for chemical compounds. *Chemical Research in Toxicology*, **2012**, 25, 2378-85	4	50
39	In silico fragment-based drug design using a PASS approach. *SAR and QSAR in Environmental Research*, **2012**, 23, 279-96	3.5	4
38	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. *Pharmaceutical Chemistry Journal*, **2012**, 45, 605-611	0.9	10
37	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. *Molecular Informatics*, **2011**, 30, 241-50	3.8	172
36	Multi-targeted natural products evaluation based on biological activity prediction with PASS. *Current Pharmaceutical Design*, **2010**, 16, 1703-17	3.3	99
35	Functional classification of proteins based on projection of amino acid sequences: application for prediction of protein kinase substrates. *BMC Bioinformatics*, **2010**, 11, 313	3.6	13
34	Collaborative development of predictive toxicology applications. *Journal of Cheminformatics*, **2010**, 2, 7	8.6	76
33	Computer-Aided Prediction of Rodent Carcinogenicity by PASS and CISOC-PSCT. *QSAR and Combinatorial Science*, **2009**, 28, 806-810		38
32	In silico method for identification of promising anticancer drug targets. *SAR and QSAR in Environmental Research*, **2009**, 20, 755-66	3.5	8
31	QNA-based 'Star Track' QSAR approach. *SAR and QSAR in Environmental Research*, **2009**, 20, 679-709	3.5	58
30	Computer-aided prediction of QT-prolongation. *SAR and QSAR in Environmental Research*, **2008**, 19, 81-90	3.5	17
29	Directions in QSAR modeling for regulatory uses in OECD member countries, EU and in Russia. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2008**, 26, 201-36	4.5	29
28	Recognition of protein function using the local similarity. *Journal of Bioinformatics and Computational Biology*, **2008**, 6, 709-25	1	6
27	Chapter 6:Probabilistic Approaches in Activity Prediction **2008**, 182-216		49
26	Computer-aided discovery of anti-inflammatory thiazolidinones with dual cyclooxygenase/lipoxygenase inhibition. *Journal of Medicinal Chemistry*, **2008**, 51, 1601-9	8.3	136

25	Prediction of biological activity profiles of cyanobacterial secondary metabolites. *SAR and QSAR in Environmental Research*, **2007**, 18, 629-43	3.5	16
24	PASS: identification of probable targets and mechanisms of toxicity. *SAR and QSAR in Environmental Research*, **2007**, 18, 101-10	3.5	71
23	A new approach to QSAR modelling of acute toxicity. *SAR and QSAR in Environmental Research*, **2007**, 18, 285-98	3.5	39
22	Prediction of protein functional specificity without an alignment. *OMICS A Journal of Integrative Biology*, **2006**, 10, 56-65	3.8	7
21	Rational design of macrolides by virtual screening of combinatorial libraries generated through in silico manipulation of polyketide synthases. *Journal of Medicinal Chemistry*, **2006**, 49, 2077-87	8.3	25
20	Computer-aided rodent carcinogenicity prediction. *Mutation Research - Genetic Toxicology and Environmental Mutagenesis*, **2005**, 586, 138-46	3	18
19	Why relevant chemical information cannot be exchanged without disclosing structures. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 705-13	4.2	13
18	Design, synthesis, computational and biological evaluation of new anxiolytics. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 6559-68	3.4	103
17	A new statistical approach to predicting aromatic hydroxylation sites. Comparison with model-based approaches. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1998-2009		28
16	Design of new cognition enhancers: from computer prediction to synthesis and biological evaluation. *Journal of Medicinal Chemistry*, **2004**, 47, 2870-6	8.3	64
15	Prediction of biological activity spectra for substances: evaluation on the diverse sets of drug-like structures. *Current Medicinal Chemistry*, **2003**, 10, 225-33	4.3	94
14	Computer-aided selection of potential antihypertensive compounds with dual mechanism of action. *Journal of Medicinal Chemistry*, **2003**, 46, 3326-32	8.3	37
13	Predicting biotransformation potential from molecular structure. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1636-46		36
12	PASS biological activity spectrum predictions in the enhanced open NCI database browser. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 228-36		159
11	Prediction of biological activity spectra via the Internet. *SAR and QSAR in Environmental Research*, **2003**, 14, 339-47	3.5	43
10	How to acquire new biological activities in old compounds by computer prediction. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 819-24	4.2	70
9	Computer-aided prediction of receptor profile for drug-like compounds. *SAR and QSAR in Environmental Research*, **2002**, 13, 433-43	3.5	4
8	Computer aided prediction of biological activity spectra: evaluating versus known and predicting of new activities for thiazole derivatives. *SAR and QSAR in Environmental Research*, **2002**, 13, 457-71	3.5	14

7	Top 200 medicines: can new actions be discovered through computer-aided prediction?. *SAR and QSAR in Environmental Research*, **2001**, 12, 327-44	3.5	40
6	Discriminating between drugs and nondrugs by prediction of activity spectra for substances (PASS). *Journal of Medicinal Chemistry*, **2001**, 44, 2432-7	8.3	101
5	Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics. *Russian Journal of Bioorganic Chemistry*, **2000**, 26, 297-305	1	1
4	PASS: prediction of activity spectra for biologically active substances. *Bioinformatics*, **2000**, 16, 747-8	7.2	511
3	Robustness of biological activity spectra predicting by computer program PASS for noncongeneric sets of chemical compounds. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1349-55		178
2	Chemical Similarity Assessment through Multilevel Neighborhoods of Atoms: Definition and Comparison with the Other Descriptors. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 666-670		143
1	Computer-Aided Estimation of Synthetic CompoundsSimilarity with Endogenous Bioregulations. *QSAR and Combinatorial Science*, **1998**, 17, 459-464		4