

Dmitry A Filimonov

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	PASS: prediction of activity spectra for biologically active substances. <i>Bioinformatics</i> , 2000 , 16, 747-8	7.2	511
95	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. <i>Chemistry of Heterocyclic Compounds</i> , 2014 , 50, 444-457	1.4	340
94	QSAR without borders. <i>Chemical Society Reviews</i> , 2020 , 49, 3525-3564	58.5	196
93	Robustness of biological activity spectra predicting by computer program PASS for noncongeneric sets of chemical compounds. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 1349-55		178
92	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. <i>Molecular Informatics</i> , 2011 , 30, 241-50	3.8	172
91	PASS biological activity spectrum predictions in the enhanced open NCI database browser. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 228-36		159
90	Chemical Similarity Assessment through Multilevel Neighborhoods of Atoms: Definition and Comparison with the Other Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 666-670		143
89	Computer-aided discovery of anti-inflammatory thiazolidinones with dual cyclooxygenase/lipoxygenase inhibition. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 1601-9	8.3	136
88	Design, synthesis, computational and biological evaluation of new anxiolytics. <i>Bioorganic and Medicinal Chemistry</i> , 2004 , 12, 6559-68	3.4	103
87	Discriminating between drugs and nondrugs by prediction of activity spectra for substances (PASS). <i>Journal of Medicinal Chemistry</i> , 2001 , 44, 2432-7	8.3	101
86	Multi-targeted natural products evaluation based on biological activity prediction with PASS. <i>Current Pharmaceutical Design</i> , 2010 , 16, 1703-17	3.3	99
85	Prediction of biological activity spectra for substances: evaluation on the diverse sets of drug-like structures. <i>Current Medicinal Chemistry</i> , 2003 , 10, 225-33	4.3	94
84	Collaborative development of predictive toxicology applications. <i>Journal of Cheminformatics</i> , 2010 , 2, 7	8.6	76
83	PASS: identification of probable targets and mechanisms of toxicity. <i>SAR and QSAR in Environmental Research</i> , 2007 , 18, 101-10	3.5	71
82	How to acquire new biological activities in old compounds by computer prediction. <i>Journal of Computer-Aided Molecular Design</i> , 2002 , 16, 819-24	4.2	70
81	Design of new cognition enhancers: from computer prediction to synthesis and biological evaluation. <i>Journal of Medicinal Chemistry</i> , 2004 , 47, 2870-6	8.3	64
80	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. <i>Biomedical Chemistry Research and Methods</i> , 2018 , 1, e00004	0.4	63

79	CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds. <i>PLoS ONE</i> , 2018 , 13, e0191838	3.7	62
78	Fragment-based design, docking, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-arylidene-4-thiazolidinones as cyclooxygenase/lipoxygenase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2012 , 47, 111-24	6.8	61
77	QNA-based 'Star Track' QSAR approach. <i>SAR and QSAR in Environmental Research</i> , 2009 , 20, 679-709	3.5	58
76	DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula. <i>Bioinformatics</i> , 2013 , 29, 2062-3	7.2	55
75	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. <i>Bioinformatics</i> , 2015 , 31, 2046-8	7.2	55
74	Quantitative prediction of antitarget interaction profiles for chemical compounds. <i>Chemical Research in Toxicology</i> , 2012 , 25, 2378-85	4	50
73	Chapter 6: Probabilistic Approaches in Activity Prediction 2008 , 182-216		49
72	Prediction of biological activity spectra via the Internet. <i>SAR and QSAR in Environmental Research</i> , 2003 , 14, 339-47	3.5	43
71	Metabolism site prediction based on xenobiotic structural formulas and PASS prediction algorithm. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 498-507	6.1	42
70	Top 200 medicines: can new actions be discovered through computer-aided prediction?. <i>SAR and QSAR in Environmental Research</i> , 2001 , 12, 327-44	3.5	40
69	A new approach to QSAR modelling of acute toxicity. <i>SAR and QSAR in Environmental Research</i> , 2007 , 18, 285-98	3.5	39
68	Computer-Aided Prediction of Rodent Carcinogenicity by PASS and CISOC-PSCT. <i>QSAR and Combinatorial Science</i> , 2009 , 28, 806-810		38
67	Computer-aided selection of potential antihypertensive compounds with dual mechanism of action. <i>Journal of Medicinal Chemistry</i> , 2003 , 46, 3326-32	8.3	37
66	Predicting biotransformation potential from molecular structure. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1636-46		36
65	ADVERPred-Web Service for Prediction of Adverse Effects of Drugs. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 8-11	6.1	34
64	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobiotics' Metabolites. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 638-642	6.1	32
63	PASS Targets: Ligand-based multi-target computational system based on a public data and naïve Bayes approach. <i>SAR and QSAR in Environmental Research</i> , 2015 , 26, 783-93	3.5	32
62	Directions in QSAR modeling for regulatory uses in OECD member countries, EU and in Russia. <i>Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews</i> , 2008 , 26, 201-36	4.5	29

61	A new statistical approach to predicting aromatic hydroxylation sites. Comparison with model-based approaches. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1998-2009		28
60	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1388-99	6.1	26
59	Rational design of macrolides by virtual screening of combinatorial libraries generated through in silico manipulation of polyketide synthases. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 2077-87	8.3	25
58	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. <i>Journal of Cheminformatics</i> , 2016 , 8, 68	8.6	19
57	Computer-aided rodent carcinogenicity prediction. <i>Mutation Research - Genetic Toxicology and Environmental Mutagenesis</i> , 2005 , 586, 138-46	3	18
56	Computer-aided prediction of xenobiotic metabolism in the human body. <i>Russian Chemical Reviews</i> , 2016 , 85, 854-879	6.8	17
55	Computer-aided prediction of QT-prolongation. <i>SAR and QSAR in Environmental Research</i> , 2008 , 19, 81-90	9.5	17
54	Online resources for the prediction of biological activity of organic compounds. <i>Russian Chemical Bulletin</i> , 2016 , 65, 384-393	1.7	16
53	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. <i>Frontiers in Chemistry</i> , 2018 , 6, 133	5	16
52	Design, synthesis and pharmacological evaluation of novel vanadium-containing complexes as antidiabetic agents. <i>PLoS ONE</i> , 2014 , 9, e100386	3.7	16
51	Prediction of biological activity profiles of cyanobacterial secondary metabolites. <i>SAR and QSAR in Environmental Research</i> , 2007 , 18, 629-43	3.5	16
50	Web Resources for Discovery and Development of New Medicines. <i>Pharmaceutical Chemistry Journal</i> , 2017 , 51, 91-99	0.9	15
49	Computer aided prediction of biological activity spectra: evaluating versus known and predicting of new activities for thiazole derivatives. <i>SAR and QSAR in Environmental Research</i> , 2002 , 13, 457-71	3.5	14
48	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. <i>Bioinformatics</i> , 2018 , 34, 710-712	7.2	13
47	Functional classification of proteins based on projection of amino acid sequences: application for prediction of protein kinase substrates. <i>BMC Bioinformatics</i> , 2010 , 11, 313	3.6	13
46	Why relevant chemical information cannot be exchanged without disclosing structures. <i>Journal of Computer-Aided Molecular Design</i> , 2005 , 19, 705-13	4.2	13
45	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. <i>Molecular Informatics</i> , 2020 , 39, e2000093	3.8	13
44	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 319-336	3	12

43	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. <i>Molecules</i> , 2018 , 23,	4.8	12
42	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. <i>Pharmaceutical Chemistry Journal</i> , 2017 , 50, 775-780	0.9	11
41	Identification of drug-induced myocardial infarction-related protein targets through the prediction of drug-target interactions and analysis of biological processes. <i>Chemical Research in Toxicology</i> , 2014 , 27, 1263-81	4	11
40	Prediction of metabolites of epoxidation reaction in MetaTox. <i>SAR and QSAR in Environmental Research</i> , 2017 , 28, 833-842	3.5	10
39	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. <i>Pharmaceutical Chemistry Journal</i> , 2012 , 45, 605-611	0.9	10
38	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. <i>Molecular Informatics</i> , 2017 , 36, 1600142	3.8	9
37	Combined network pharmacology and virtual reverse pharmacology approaches for identification of potential targets to treat vascular dementia. <i>Scientific Reports</i> , 2020 , 10, 257	4.9	9
36	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4513-4518	6.1	9
35	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of K and IC Values of Antitarget Inhibitors. <i>Frontiers in Pharmacology</i> , 2018 , 9, 1136	5.6	9
34	Data Mining Approach for Extraction of Useful Information About Biologically Active Compounds from Publications. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3635-3644	6.1	8
33	Drug-drug interaction prediction using PASS. <i>SAR and QSAR in Environmental Research</i> , 2019 , 30, 655-664	3.5	8
32	Identification of drug targets related to the induction of ventricular tachyarrhythmia through a systems chemical biology approach. <i>Toxicological Sciences</i> , 2015 , 145, 321-36	4.4	8
31	In silico method for identification of promising anticancer drug targets. <i>SAR and QSAR in Environmental Research</i> , 2009 , 20, 755-66	3.5	8
30	Metatox - Web application for generation of metabolic pathways and toxicity estimation. <i>Journal of Bioinformatics and Computational Biology</i> , 2019 , 17, 1940001	1	8
29	PASS-based approach to predict HIV-1 reverse transcriptase resistance. <i>Journal of Bioinformatics and Computational Biology</i> , 2017 , 15, 1650040	1	7
28	Prediction of protein functional specificity without an alignment. <i>OMICS A Journal of Integrative Biology</i> , 2006 , 10, 56-65	3.8	7
27	Integral estimation of xenobiotics toxicity with regard to their metabolism in human organism. <i>Pure and Applied Chemistry</i> , 2017 , 89, 1449-1458	2.1	7
26	Prediction of Protein-Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. <i>International Journal of Molecular Sciences</i> , 2019 , 21,	6.3	7

25	Data and Text Mining Help Identify Key Proteins Involved in the Molecular Mechanisms Shared by SARS-CoV-2 and HIV-1. <i>Molecules</i> , 2020 , 25,	4.8	6
24	A Computational Approach for the Prediction of Treatment History and the Effectiveness or Failure of Antiretroviral Therapy. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	6
23	Recognition of protein function using the local similarity. <i>Journal of Bioinformatics and Computational Biology</i> , 2008 , 6, 709-25	1	6
22	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. <i>Molecules</i> , 2019 , 24,	4.8	6
21	QNA-Based Prediction of Sites of Metabolism. <i>Molecules</i> , 2017 , 22,	4.8	5
20	Assessment of the cardiovascular adverse effects of drug-drug interactions through a combined analysis of spontaneous reports and predicted drug-target interactions. <i>PLoS Computational Biology</i> , 2019 , 15, e1006851	5	5
19	Computer-Aided Estimation of Biological Activity Profiles of Drug-Like Compounds Taking into Account Their Metabolism in Human Body. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	5
18	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. <i>Bioinformatics</i> , 2020 , 36, 978-979	7.2	5
17	PASS-based prediction of metabolites detection in biological systems. <i>SAR and QSAR in Environmental Research</i> , 2019 , 30, 751-758	3.5	4
16	Prediction of amino acid positions specific for functional groups in a protein family based on local sequence similarity. <i>Journal of Molecular Recognition</i> , 2016 , 29, 159-69	2.6	4
15	In silico fragment-based drug design using a PASS approach. <i>SAR and QSAR in Environmental Research</i> , 2012 , 23, 279-96	3.5	4
14	Computer-aided prediction of receptor profile for drug-like compounds. <i>SAR and QSAR in Environmental Research</i> , 2002 , 13, 433-43	3.5	4
13	In Silico Prediction of Drug-Drug Interactions Mediated by Cytochrome P450 Isoforms. <i>Pharmaceutics</i> , 2021 , 13,	6.4	4
12	Computer-Aided Estimation of Synthetic Compounds Similarity with Endogenous Bioregulations. <i>QSAR and Combinatorial Science</i> , 1998 , 17, 459-464		4
11	Virtual Screening for Potential Substances for the Prophylaxis of HIV Infection in Libraries of Commercially Available Organic Compounds. <i>Pharmaceutical Chemistry Journal</i> , 2013 , 47, 343-360	0.9	3
10	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. <i>Molecules</i> , 2019 , 25,	4.8	2
9	Prediction of Protein-ligand Interaction Based on Sequence Similarity and Ligand Structural Features. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	2
8	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. <i>Molecular Informatics</i> , 2021 , 40, e2000231	3.8	2

7	Improving (Q)SAR predictions by examining bias in the selection of compounds for experimental testing. <i>SAR and QSAR in Environmental Research</i> , 2019 , 30, 759-773	3.5	1
6	Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics. <i>Russian Journal of Bioorganic Chemistry</i> , 2000 , 26, 297-305	1	1
5	Capacities of computer evaluation of hidden potential of phytochemicals of medicinal plants of the traditional Indian Ayurvedic medicine. <i>Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry</i> , 2016 , 10, 43-54	0.4	1
4	Machine Learning Methods in Antiviral Drug Discovery. <i>Topics in Medicinal Chemistry</i> , 2021 , 245-279	0.4	0
3	Extraction of Data on Parent Compounds and Their Metabolites from Texts of Scientific Abstracts. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 1683-1690	6.1	0
2	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain.. <i>Computational Biology and Chemistry</i> , 2022 , 98, 107674	3.6	0
1	TCR-PRED [WEB SERVICE FOR PREDICTING THE SPECIFICITY OF EPITOPES FOR TCR CDR3 SEQUENCES BASED ON THEIR STRUCTURAL FORMULAS 2021 , 1, 212-214	0	