

V V Poroikov

List of Publications by Year in descending order

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221
papers

8,457
citations

61977

43
h-index

58576

82
g-index

262
all docs

262
docs citations

262
times ranked

7116
citing authors

#	ARTICLE	IF	CITATIONS
1	PASS: prediction of activity spectra for biologically active substances. <i>Bioinformatics</i> , 2000, 16, 747-748.	4.1	737
2	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.	1.2	630
3	QSAR without borders. <i>Chemical Society Reviews</i> , 2020, 49, 3525-3564.	38.1	427
4	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. <i>Molecular Informatics</i> , 2011, 30, 241-250.	2.5	278
5	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, 1349-1355.	2.8	217
6	PASS Biological Activity Spectrum Predictions in the Enhanced Open NCI Database Browser. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 228-236.	2.8	203
7	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.	2.8	192
8	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1601-1609.	6.4	161
9	PASS-assisted exploration of new therapeutic potential of natural products. <i>Medicinal Chemistry Research</i> , 2011, 20, 1509-1514.	2.4	134
10	A critical overview of computational approaches employed for COVID-19 drug discovery. <i>Chemical Society Reviews</i> , 2021, 50, 9121-9151.	38.1	128
11	Multi-Targeted Natural Products Evaluation Based on Biological Activity Prediction with PASS. <i>Current Pharmaceutical Design</i> , 2010, 16, 1703-1717.	1.9	126
12	Discriminating between Drugs and Nondrugs by Prediction of Activity Spectra for Substances (PASS). <i>Journal of Medicinal Chemistry</i> , 2001, 44, 2432-2437.	6.4	124
13	Cyclobutane-Containing Alkaloids: Origin, Synthesis, and Biological Activities. <i>Open Medicinal Chemistry Journal</i> , 2008, 2, 26-37.	2.4	121
14	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020, 128, 27002.	6.0	120
15	Prediction of Biological Activity Spectra for Substances: Evaluation on the Diverse Sets of Drug-Like Structures. <i>Current Medicinal Chemistry</i> , 2003, 10, 225-233.	2.4	117
16	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.	2.5	116
17	Design, synthesis, computational and biological evaluation of new anxiolytics. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 6559-6568.	3.0	114
18	Novel Antitumor Agents: Marine Sponge Alkaloids, their Synthetic Analogs and Derivatives. <i>Mini-Reviews in Medicinal Chemistry</i> , 2005, 5, 319-336.	2.4	106

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19	Natural Peroxy Anticancer Agents. Mini-Reviews in Medicinal Chemistry, 2007, 7, 571-589.	2.4	106
20	Chemo- and bioinformatics resources for <i>in silico</i> drug discovery from medicinal plants beyond their traditional use: a critical review. Natural Product Reports, 2014, 31, 1585-1611.	10.3	104
21	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. Biomedical Chemistry Research and Methods, 2018, 1, e00004.	0.4	99
22	PASS: identification of probable targets and mechanisms of toxicity. SAR and QSAR in Environmental Research, 2007, 18, 101-110.	2.2	95
23	Ameliorative effect of Curcumin on seizure severity, depression like behavior, learning and memory deficit in post-pentylenetetrazole-kindled mice. European Journal of Pharmacology, 2013, 704, 33-40.	3.5	93
24	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	6.1	91
25	DIGEP-Pred: web service for <i>in silico</i> prediction of drug-induced gene expression profiles based on structural formula. Bioinformatics, 2013, 29, 2062-2063.	4.1	87
26	QNA-based <i>Star Track</i> ™ QSAR approach. SAR and QSAR in Environmental Research, 2009, 20, 679-709.	2.2	84
27	How to acquire new biological activities in old compounds by computer prediction. Journal of Computer-Aided Molecular Design, 2002, 16, 819-824.	2.9	83
28	SOMP: web server for <i>in silico</i> prediction of sites of metabolism for drug-like compounds. Bioinformatics, 2015, 31, 2046-2048.	4.1	83
29	Design of New Cognition Enhancers: From Computer Prediction to Synthesis and Biological Evaluation. Journal of Medicinal Chemistry, 2004, 47, 2870-2876.	6.4	75
30	Fragment-based design, docking, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-arylidene-4-thiazolidinones as cyclooxygenase/lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2012, 47, 111-124.	5.5	72
31	Naturally occurring plant isoquinoline N-oxide alkaloids: Their pharmacological and SAR activities. Phytomedicine, 2015, 22, 183-202.	5.3	72
32	Quantitative Prediction of Antitarget Interaction Profiles for Chemical Compounds. Chemical Research in Toxicology, 2012, 25, 2378-2385.	3.3	70
33	Probabilistic Approaches in Activity Prediction. , 2008, , 182-216.		67
34	QSAR Modeling and Prediction of Drug-Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
35	Computational platform Way2Drug: from the prediction of biological activity to drug repurposing. Russian Chemical Bulletin, 2017, 66, 1832-1841.	1.5	60
36	Prediction of Biological Activity Spectra via The Internet. SAR and QSAR in Environmental Research, 2003, 14, 339-347.	2.2	56

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37	Computer-aided prediction of biological activity spectra for organic compounds: the possibilities and limitations. <i>Russian Chemical Bulletin</i> , 2019, 68, 2143-2154.	1.5	56
38	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, 783-793.	2.2	52
39	In silico assessment of adverse drug reactions and associated mechanisms. <i>Drug Discovery Today</i> , 2016, 21, 58-71.	6.4	51
40	How good are publicly available web services that predict bioactivity profiles for drug repurposing?. <i>SAR and QSAR in Environmental Research</i> , 2017, 28, 843-862.	2.2	51
41	Top 200 Medicines: Can New Actions be Discovered Through Computer-aided Prediction?. <i>SAR and QSAR in Environmental Research</i> , 2001, 12, 327-344.	2.2	50
42	Metabolism Site Prediction Based on Xenobiotic Structural Formulas and PASS Prediction Algorithm. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 498-507.	5.4	50
43	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobiotics'™ Metabolites. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 638-642.	5.4	50
44	ADVERPred'™ Web Service for Prediction of Adverse Effects of Drugs. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 8-11.	5.4	50
45	A new approach to QSAR modelling of acute toxicity'™. <i>SAR and QSAR in Environmental Research</i> , 2007, 18, 285-298.	2.2	49
46	Computer-aided prediction for medicinal chemistry via the Internet. <i>SAR and QSAR in Environmental Research</i> , 2008, 19, 27-38.	2.2	44
47	Pharmacological and Predicted Activities of Natural Azo Compounds. <i>Natural Products and Bioprospecting</i> , 2017, 7, 151-169.	4.3	44
48	Computer-Aided Prediction of Rodent Carcinogenicity by PASS and CISOC'™PSCT. <i>QSAR and Combinatorial Science</i> , 2009, 28, 806-810.	1.4	43
49	Evaluation of the local anaesthetic activity of 3-aminobenzo[d]isothiazole derivatives using the rat sciatic nerve model. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 473-481.	5.5	43
50	Computer-Aided Selection of Potential Antihypertensive Compounds with Dual Mechanism of Action. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 3326-3332.	6.4	40
51	Predicting Biotransformation Potential from Molecular Structure. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1636-1646.	2.8	40
52	Molecular Docking Studies of HIV-1 Resistance to Reverse Transcriptase Inhibitors: Mini-Review. <i>Molecules</i> , 2018, 23, 1233.	3.8	37
53	Synthesis and anticancer activity of quinopimaric and maleopimaric acids'™ derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 6481-6489.	3.0	36
54	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, 201-236.	2.9	35

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55	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1388-1399.	5.4	34
56	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.	2.8	31
57	Revealing pharmacodynamics of medicinal plants using in silico approach: A case study with wet lab validation. <i>Computers in Biology and Medicine</i> , 2014, 47, 1-6.	7.0	31
58	Multi-omics "upstream analysis" of regulatory genomic regions helps identifying targets against methotrexate resistance of colon cancer. <i>EuPA Open Proteomics</i> , 2016, 13, 1-13.	2.5	31
59	Synthesis, antifungal activity and QSAR study of 2-arylhydroxynitroindoles. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 4374-4382.	5.5	30
60	Naturally occurring aromatic steroids and their biological activities. <i>Applied Microbiology and Biotechnology</i> , 2018, 102, 4663-4674.	3.6	29
61	The synthesis and hepatoprotective activity of esters of the lupane group triterpenoids. <i>Russian Journal of Bioorganic Chemistry</i> , 2000, 26, 192-200.	1.0	28
62	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, 2077-2087.	6.4	28
63	Pharmacological profile of natural and synthetic compounds with rigid adamantane-based scaffolds as potential agents for the treatment of neurodegenerative diseases. <i>Biochemical and Biophysical Research Communications</i> , 2020, 529, 1225-1241.	2.1	28
64	Computer-aided prediction of QT-prolongation. SAR and QSAR in Environmental Research, 2008, 19, 81-90.	2.2	27
65	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. <i>Frontiers in Chemistry</i> , 2018, 6, 133.	3.6	27
66	Chemical Diversity of Soft Coral Steroids and Their Pharmacological Activities. <i>Marine Drugs</i> , 2020, 18, 613.	4.6	27
67	Anticonvulsant activity and acute neurotoxic profile of <i>Achyranthes aspera</i> Linn.. <i>Journal of Ethnopharmacology</i> , 2017, 202, 97-102.	4.1	26
68	Derivatives of Piperazines as Potential Therapeutic Agents for Alzheimer's Disease. <i>Molecular Pharmacology</i> , 2019, 95, 337-348.	2.3	26
69	Comparative analysis of amino acid sequences from envelope proteins isolated from different hepatitis C virus variants: possible role of conservative and variable regions. <i>Journal of Viral Hepatitis</i> , 2000, 7, 368-374.	2.0	25
70	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. <i>Molecules</i> , 2018, 23, 2751.	3.8	25
71	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. <i>Journal of Cheminformatics</i> , 2016, 8, 68.	6.1	24
72	Computer-aided prediction and cytotoxicity evaluation of dithiocarbamates of 9,10-anthracenedione as new anticancer agents. SAR and QSAR in Environmental Research, 2017, 28, 355-366.	2.2	24

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73	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. <i>Bioinformatics</i> , 2018, 34, 710-712.	4.1	24
74	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4513-4518.	5.4	24
75	Highly oxygenated isoprenoid lipids derived from fungi and fungal endophytes: Origin and biological activities. <i>Steroids</i> , 2018, 140, 114-124.	1.8	23
76	Computer-aided prediction of xenobiotic metabolism in the human body. <i>Russian Chemical Reviews</i> , 2016, 85, 854-879.	6.5	22
77	Online resources for the prediction of biological activity of organic compounds. <i>Russian Chemical Bulletin</i> , 2016, 65, 384-393.	1.5	22
78	Hydroperoxy steroids and triterpenoids derived from plant and fungi: Origin, structures and biological activities. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2019, 190, 76-87.	2.5	22
79	Molecular Mechanisms of Protein-Protein Recognition: Whether the Surface Placed Charged Residues determine the Recognition Process?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2001, 19, 279-284.	3.5	21
80	Computer-aided rodent carcinogenicity prediction. <i>Mutation Research - Genetic Toxicology and Environmental Mutagenesis</i> , 2005, 586, 138-146.	1.7	21
81	OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia. <i>Journal of Biomedical Semantics</i> , 2012, 3, S7.	1.6	21
82	Peroxy steroids derived from plant and fungi and their biological activities. <i>Applied Microbiology and Biotechnology</i> , 2018, 102, 7657-7667.	3.6	21
83	The Method of Self-Consistent Regression for the Quantitative Analysis of Relationships Between Structure and Properties of Chemicals. <i>Pharmaceutical Chemistry Journal</i> , 2004, 38, 21-24.	0.8	20
84	A QSAR and molecular modelling study towards new lead finding: polypharmacological approach to <i>Mycobacterium tuberculosis</i> . <i>SAR and QSAR in Environmental Research</i> , 2017, 28, 815-832.	2.2	20
85	Structural-Functional Analysis of 2,1,3-Benzoxadiazoles and Their N-oxides As HIV-1 Integrase Inhibitors. <i>Acta Naturae</i> , 2013, 5, 63-72.	1.7	20
86	Computer Aided Predicting the Biological Activity Spectra and Experimental Testing of New Thiazole Derivatives. <i>QSAR and Combinatorial Science</i> , 1999, 18, 16-25.	1.2	19
87	Fragment-based lead design. <i>Russian Chemical Reviews</i> , 2012, 81, 158-174.	6.5	19
88	Drug-drug interaction prediction using PASS. <i>SAR and QSAR in Environmental Research</i> , 2019, 30, 655-664.	2.2	19
89	Prediction of Protein-Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. <i>International Journal of Molecular Sciences</i> , 2020, 21, 24.	4.1	19
90	Antibacterial activity of griseofulvin analogues as an example of drug repurposing. <i>International Journal of Antimicrobial Agents</i> , 2020, 55, 105884.	2.5	19

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91	Synthesis and anticancer activity of aminopropoxytriterpenoids. <i>Medicinal Chemistry Research</i> , 2015, 24, 3423-3436.	2.4	18
92	Revealing Medicinal Plants That Are Useful for the Comprehensive Management of Epilepsy and Associated Comorbidities through In Silico Mining of Their Phytochemical Diversity. <i>Planta Medica</i> , 2015, 81, 495-506.	1.3	18
93	Synthesis and chemoinformatics analysis of N-aryl- β -alanine derivatives. <i>Research on Chemical Intermediates</i> , 2015, 41, 7517-7540.	2.7	18
94	Web Resources for Discovery and Development of New Medicines. <i>Pharmaceutical Chemistry Journal</i> , 2017, 51, 91-99.	0.8	18
95	Etoposide-Induced Apoptosis in Cancer Cells Can Be Reinforced by an Uncoupled Link between Hsp70 and Caspase-3. <i>International Journal of Molecular Sciences</i> , 2018, 19, 2519.	4.1	18
96	HIV Resistance Prediction to Reverse Transcriptase Inhibitors: Focus on Open Data. <i>Molecules</i> , 2018, 23, 956.	3.8	18
97	Novel antimicrobial agentsâ€™ discovery among the steroid derivatives. <i>Steroids</i> , 2019, 144, 52-65.	1.8	18
98	New Caffeic Acid Derivatives as Antimicrobial Agents: Design, Synthesis, Evaluation and Docking. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 292-304.	2.1	18
99	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, 457-471.	2.2	17
100	Why relevant chemical information cannot be exchanged without disclosing structures. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 705-713.	2.9	17
101	Prediction of biological activity profiles of cyanobacterial secondary metabolites. <i>SAR and QSAR in Environmental Research</i> , 2007, 18, 629-643.	2.2	17
102	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. <i>PLoS ONE</i> , 2014, 9, e100386.	2.5	17
103	Computer-aided design and discovery of proteinâ€“protein interaction inhibitors as agents for anti-HIV therapy. <i>SAR and QSAR in Environmental Research</i> , 2014, 25, 457-471.	2.2	17
104	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of Ki and IC50 Values of Antitarget Inhibitors. <i>Frontiers in Pharmacology</i> , 2018, 9, 1136.	3.5	17
105	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, 7492.	4.1	17
106	The Sistemax Web Portal of Natural Products: An Update. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2516-2522.	5.4	17
107	Triazolo Based-Thiadiazole Derivatives. Synthesis, Biological Evaluation and Molecular Docking Studies. <i>Antibiotics</i> , 2021, 10, 804.	3.7	17
108	CYCLONET--an integrated database on cell cycle regulation and carcinogenesis. <i>Nucleic Acids Research</i> , 2007, 35, D550-D556.	14.5	16

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109	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. <i>Pharmaceutical Chemistry Journal</i> , 2017, 50, 775-780.	0.8	16
110	Pharmacological repositioning of <i>Achyranthes aspera</i> as an antidepressant using pharmacoinformatic tools PASS and PharmaExpert: a case study with wet lab validation. <i>SAR and QSAR in Environmental Research</i> , 2018, 29, 69-81.	2.2	16
111	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.	5.4	16
112	3-Amino-5-(indol-3-yl)methylene-4-oxo-2-thioxothiazolidine Derivatives as Antimicrobial Agents: Synthesis, Computational and Biological Evaluation. <i>Pharmaceuticals</i> , 2020, 13, 229.	3.8	16
113	Computer Design of Vaccines: Approaches, Software Tools and Informational Resources. <i>Current Computer-Aided Drug Design</i> , 2005, 1, 207-222.	1.2	15
114	PASS-based approach to predict HIV-1 reverse transcriptase resistance. <i>Journal of Bioinformatics and Computational Biology</i> , 2017, 15, 1650040.	0.8	15
115	Molecular property diagnostic suite for diabetes mellitus (MPDSDM): An integrated web portal for drug discovery and drug repurposing. <i>Journal of Biomedical Informatics</i> , 2018, 85, 114-125.	4.3	15
116	Naturally occurring of β , γ -diepoxy-containing compounds: origin, structures, and biological activities. <i>Applied Microbiology and Biotechnology</i> , 2019, 103, 3249-3264.	3.6	15
117	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. <i>Molecules</i> , 2019, 24, 3955.	3.8	15
118	Antihypoxic Action of <i>Panax Japonicus</i> , <i>Tribulus Terrestris</i> and <i>Dioscorea Deltoidea</i> Cell Cultures: In Silico and Animal Studies. <i>Molecular Informatics</i> , 2020, 39, e2000093.	2.5	15
119	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.	2.1	15
120	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.	2.6	14
121	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, 1263-1281.	3.3	14
122	Novel HIV-1 Integrase Inhibitor Development by Virtual Screening Based on QSAR Models. <i>Current Topics in Medicinal Chemistry</i> , 2015, 16, 441-448.	2.1	14
123	Antiprotozoal and Antitumor Activity of Natural Polycyclic Endoperoxides: Origin, Structures and Biological Activity. <i>Molecules</i> , 2021, 26, 686.	3.8	14
124	Pass. , 2005, , 459-478.		14
125	Computer-aided prediction of activity spectrum for substance (PASS) system evaluated on a set of new biologically active compounds. <i>Pharmaceutical Chemistry Journal</i> , 1998, 32, 658-664.	0.8	13
126	Metatox - Web application for generation of metabolic pathways and toxicity estimation. <i>Journal of Bioinformatics and Computational Biology</i> , 2019, 17, 1940001.	0.8	13

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127	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, 748.	4.1	13
128	Endocrine disruption profile analysis of 11,416 chemicals from chemometrical tools. SAR and QSAR in <i>Environmental Research</i> , 2007, 18, 181-193.	2.2	12
129	In silico method for identification of promising anticancer drug targets. SAR and QSAR in <i>Environmental Research</i> , 2009, 20, 755-766.	2.2	12
130	Computer Evaluation of Drug Interactions with P-Glycoprotein. <i>Bulletin of Experimental Biology and Medicine</i> , 2013, 154, 521-524.	0.8	12
131	<i>In Silico</i> Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. <i>Molecular Informatics</i> , 2017, 36, 1600142.	2.5	12
132	Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in <i>Environmental Research</i> , 2017, 28, 833-842.	2.2	12
133	Naturally occurring marine 1,2-epoxy steroids: Origin and biological activities. <i>Vietnam Journal of Chemistry</i> , 2018, 56, 409-433.	0.8	12
134	Computer-Aided Drug Design: from Discovery of Novel Pharmaceutical Agents to Systems Pharmacology. <i>Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry</i> , 2020, 14, 216-227.	0.4	12
135	Antimicrobial Activity of Nitrogen-Containing 5- α -Androstane Derivatives: In Silico and Experimental Studies. <i>Antibiotics</i> , 2020, 9, 224.	3.7	12
136	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, 2944.	3.8	12
137	Molecular descriptor analysis of approved drugs using unsupervised learning for drug repurposing. <i>Computers in Biology and Medicine</i> , 2021, 138, 104856.	7.0	12
138	Computer-aided prediction of prodrug activity using the pass system. <i>Pharmaceutical Chemistry Journal</i> , 1996, 30, 760-763.	0.8	11
139	Computerized Prediction, Synthesis, and Antimicrobial Activity of New Amino-Acid Derivatives of 2-Chloro-N-(9,10-Dioxo-9,10-Dihydroanthracen-1-yl)Acetamide. <i>Pharmaceutical Chemistry Journal</i> , 2014, 48, 582-586.	0.8	11
140	Identification of Drug Targets Related to the Induction of Ventricular Tachyarrhythmia Through a Systems Chemical Biology Approach. <i>Toxicological Sciences</i> , 2015, 145, 321-336.	3.1	11
141	Molecular property diagnostic suite (MPDS): Development of disease-specific open source web portals for drug discovery. SAR and QSAR in <i>Environmental Research</i> , 2017, 28, 913-926.	2.2	11
142	Study of local anesthetic activity of some derivatives of 3-amino-BENZO-[d]-Isothiazole. SAR and QSAR in <i>Environmental Research</i> , 2003, 14, 485-495.	2.2	10
143	Acetylenic Aquatic Anticancer Agents and Related Compounds. <i>Natural Product Communications</i> , 2006, 1, 1934578X0600100.	0.5	10
144	Quantum chemical simulation of cytochrome P450 catalyzed aromatic oxidation: Metabolism, toxicity, and biodegradation of benzene derivatives. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2454-2478.	2.0	10

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145	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. <i>Pharmaceutical Chemistry Journal</i> , 2012, 45, 605-611.	0.8	10
146	Identification of potential drug targets for treatment of refractory epilepsy using network pharmacology. <i>Journal of Bioinformatics and Computational Biology</i> , 2018, 16, 1840002.	0.8	10
147	PASS-based prediction of metabolites detection in biological systems. <i>SAR and QSAR in Environmental Research</i> , 2019, 30, 751-758.	2.2	10
148	9,10-Anthraquinone Dithiocarbamates as Potential Pharmaceutical Substances with Pleiotropic Actions: Computerized Prediction of Biological Activity and Experimental Validation. <i>Pharmaceutical Chemistry Journal</i> , 2020, 53, 905-913.	0.8	10
149	Prediction of Protein Functional Specificity without an Alignment. <i>OMICS A Journal of Integrative Biology</i> , 2006, 10, 56-65.	2.0	9
150	Virtual screening of chemical compounds active against breast cancer cell lines based on cell cycle modelling, prediction of cytotoxicity and interaction with targets. <i>SAR and QSAR in Environmental Research</i> , 2015, 26, 595-604.	2.2	9
151	AntiHIV-Pred: web-resource for <i>in silico</i> prediction of anti-HIV/AIDS activity. <i>Bioinformatics</i> , 2020, 36, 978-979.	4.1	9
152	Using systems medicine to identify a therapeutic agent with potential for repurposing in inflammatory bowel disease. <i>DMM Disease Models and Mechanisms</i> , 2020, 13, .	2.4	9
153	In Silico Prediction of Drug-Drug Interactions Mediated by Cytochrome P450 Isoforms. <i>Pharmaceutics</i> , 2021, 13, 538.	4.5	9
154	Phytochemical Analysis of Polyphenol Secondary Metabolites in Cloudberry (<i>Rubus Chamaemorus L.</i>) Leaves. <i>Pharmaceutical Chemistry Journal</i> , 2021, 55, 253-258.	0.8	9
155	RECOGNITION OF PROTEIN FUNCTION USING THE LOCAL SIMILARITY. <i>Journal of Bioinformatics and Computational Biology</i> , 2008, 06, 709-725.	0.8	8
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