V V Poroikov

List of Publications by Year
in descending order

221 papers	8,457 citations	61984 43 h-index	58581 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. Bioinformatics, 2000, 16, 747-748.	4.1	737
2	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. Chemistry of Heterocyclic Compounds, 2014, 50, 444-457.	1.2	630
3	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
4	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. Molecular Informatics, 2011, 30, 241-250.	2.5	278
5	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, 1349-1355.	2.8	217
6	PASS Biological Activity Spectrum Predictions in the Enhanced Open NCI Database Browser. Journal of Chemical Information and Computer Sciences, 2003, 43, 228-236.	2.8	203
7	Chemical Similarity Assessment through Multilevel Neighborhoods of Atoms:â€‰ Definition and Comparison with the Other Descriptors. Journal of Chemical Information and Computer Sciences, 1999, 39, 666-670.	2.8	192
8	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. Journal of Medicinal Chemistry, 2008, 51, 1601-1609.	6.4	161
9	PASS-assisted exploration of new therapeutic potential of natural products. Medicinal Chemistry Research, 2011, 20, 1509-1514.	2.4	134
10	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
11	Multi-Targeted Natural Products Evaluation Based on Biological Activity Prediction with PASS. Current Pharmaceutical Design, 2010, 16, 1703-1717.	1.9	126
12	Discriminating between Drugs and Nondrugs by Prediction of Activity Spectra for Substances (PASS). Journal of Medicinal Chemistry, 2001, 44, 2432-2437.	6.4	124
13	Cyclobutane-Containing Alkaloids: Origin, Synthesis, and Biological Activities. Open Medicinal Chemistry Journal, 2008, 2, 26-37.	2.4	121
14	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
15	Prediction of Biological Activity Spectra for Substances: Evaluation on the Diverse Sets of Drug-Like Structures. Current Medicinal Chemistry, 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. PLoS ONE, 2018, 13, e0191838.	2.5	116
17	Design, synthesis, computational and biological evaluation of new anxiolytics. Bioorganic and Medicinal Chemistry, 2004, 12, 6559-6568.	3.0	114
18	Novel Antitumor Agents: Marine Sponge Alkaloids, their Synthetic Analogs and Derivatives. Mini-Reviews in Medicinal Chemistry, 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 inÂsilico 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 in silico prediction of drug-induced gene expression profiles based on structural formula. Bioinformatics, 2013, 29, 2062-2063.	4.1	87
26	QNA-based â€˜Star Trackâ€™ 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 in silico prediction of sites of metabolism for drug-like compounds. Bioinformatics, 2015, 31, 2046-2048.	4.1	83
29	Design of New Cognition Enhancers:â€‰ 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 structureâ€“activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/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 Drugâ€“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. Russian Chemical Bulletin, 2019, 68, 2143-2154.	1.5	56
38	PASS Targets: Ligand-based multi-target computational system based on a public data and naÃ¯ve Bayes approach. SAR and QSAR in Environmental Research, 2015, 26, 783-793.	2.2	52
39	In silico assessment of adverse drug reactions and associated mechanisms. Drug Discovery Today, 2016, 21, 58-71.	6.4	51
40	How good are publicly available web services that predict bioactivity profiles for drug repurposing?. SAR and QSAR in Environmental Research, 2017, 28, 843-862.	2.2	51
41	Top 200 Medicines: Can New Actions be Discovered Through Computer-aided Prediction?. SAR and QSAR in Environmental Research, 2001, 12, 327-344.	2.2	50
42	Metabolism Site Prediction Based on Xenobiotic Structural Formulas and PASS Prediction Algorithm. Journal of Chemical Information and Modeling, 2014, 54, 498-507.	5.4	50
43	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobioticsâ€™ Metabolites. Journal of Chemical Information and Modeling, 2017, 57, 638-642.	5.4	50
44	ADVERPredâ€“Web Service for Prediction of Adverse Effects of Drugs. Journal of Chemical Information and Modeling, 2018, 58, 8-11.	5.4	50
45	A new approach to QSAR modelling of acute toxicityâ€. SAR and QSAR in Environmental Research, 2007, 18, 285-298.	2.2	49
46	Computer-aided prediction for medicinal chemistry via the Internet. SAR and QSAR in Environmental Research, 2008, 19, 27-38.	2.2	44
47	Pharmacological and Predicted Activities of Natural Azo Compounds. Natural Products and Bioprospecting, 2017, 7, 151-169.	4.3	44
48	Computerâ€Aided Prediction of Rodent Carcinogenicity by PASS and CISOCâ€PSCT. QSAR and Combinatorial Science, 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. European Journal of Medicinal Chemistry, 2009, 44, 473-481.	5.5	43
50	Computer-Aided Selection of Potential Antihypertensive Compounds with Dual Mechanism of Action. Journal of Medicinal Chemistry, 2003, 46, 3326-3332.	6.4	40
51	Predicting Biotransformation Potential from Molecular Structure. Journal of Chemical Information and Computer Sciences, 2003, 43, 1636-1646.	2.8	40
52	Molecular Docking Studies of HIV-1 Resistance to Reverse Transcriptase Inhibitors: Mini-Review. Molecules, 2018, 23, 1233.	3.8	37
53	Synthesis and anticancer activity of quinopimaric and maleopimaric acidsâ€™ derivatives. Bioorganic and Medicinal Chemistry, 2014, 22, 6481-6489.	3.0	36
54	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, 201-236.	2.9	35

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55	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1388-1399.	5.4	34
56	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.	2.8	31
57	Revealing pharmacodynamics of medicinal plants using in silico approach: A case study with wet lab validation. Computers in Biology and Medicine, 2014, 47, 1-6.	7.0	31
58	Multi-omics â€œupstream analysisâ€•of regulatory genomic regions helps identifying targets against methotrexate resistance of colon cancer. EuPA Open Proteomics, 2016, 13, 1-13.	2.5	31
59	Synthesis, antifungal activity and QSAR study of 2-arylhydroxynitroindoles. European Journal of Medicinal Chemistry, 2011, 46, 4374-4382.	5.5	30
60	Naturally occurring aromatic steroids and their biological activities. Applied Microbiology and Biotechnology, 2018, 102, 4663-4674.	3.6	29
61	The synthesis and hepatoprotective activity of esters of the lupane group triterpenoids. Russian Journal of Bioorganic Chemistry, 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. Journal of Medicinal Chemistry, 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. Biochemical and Biophysical Research Communications, 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. Frontiers in Chemistry, 2018, 6, 133.	3.6	27
66	Chemical Diversity of Soft Coral Steroids and Their Pharmacological Activities. Marine Drugs, 2020, 18, 613.	4.6	27
67	Anticonvulsant activity and acute neurotoxic profile of Achyranthes aspera Linn.. Journal of Ethnopharmacology, 2017, 202, 97-102.	4.1	26
68	Derivatives of Piperazines as Potential Therapeutic Agents for Alzheimerâ€™s Disease. Molecular Pharmacology, 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. Journal of Viral Hepatitis, 2000, 7, 368-374.	2.0	25
70	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. Molecules, 2018, 23, 2751.	3.8	25
71	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. Journal of Cheminformatics, 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. Bioinformatics, 2018, 34, 710-712.	4.1	24
74	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. Journal of Chemical Information and Modeling, 2019, 59, 4513-4518.	5.4	24
75	Highly oxygenated isoprenoid lipids derived from fungi and fungal endophytes: Origin and biological activities. Steroids, 2018, 140, 114-124.	1.8	23
76	Computer-aided prediction of xenobiotic metabolism in the human body. Russian Chemical Reviews, 2016, 85, 854-879.	6.5	22
77	Online resources for the prediction of biological activity of organic compounds. Russian Chemical Bulletin, 2016, 65, 384-393.	1.5	22
78	Hydroperoxy steroids and triterpenoids derived from plant and fungi: Origin, structures and biological activities. Journal of Steroid Biochemistry and Molecular Biology, 2019, 190, 76-87.	2.5	22
79	Molecular Mechanisms of Protein-Protein Recognition: Whether the Surface Placed Charged Residues determine the Recognition Process?. Journal of Biomolecular Structure and Dynamics, 2001, 19, 279-284.	3.5	21
80	Computer-aided rodent carcinogenicity prediction. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2005, 586, 138-146.	1.7	21
81	OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia. Journal of Biomedical Semantics, 2012, 3, S7.	1.6	21
82	Peroxy steroids derived from plant and fungi and their biological activities. Applied Microbiology and Biotechnology, 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. Pharmaceutical Chemistry Journal, 2004, 38, 21-24.	0.8	20
84	A QSAR and molecular modelling study towards new lead finding: polypharmacological approach to Mycobacterium tuberculosis. SAR and QSAR in Environmental Research, 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. Acta Naturae, 2013, 5, 63-72.	1.7	20
86	Computer Aided Predicting the Biological Activity Spectra and Experimental Testing of New Thiazole Derivatives. QSAR and Combinatorial Science, 1999, 18, 16-25.	1.2	19
87	Fragment-based lead design. Russian Chemical Reviews, 2012, 81, 158-174.	6.5	19
88	Drug-drug interaction prediction using PASS. SAR and QSAR in Environmental Research, 2019, 30, 655-664.	2.2	19
89	Prediction of Proteinâ€“Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. International Journal of Molecular Sciences, 2020, 21, 24.	4.1	19
90	Antibacterial activity of griseofulvin analogues as an example of drug repurposing. International Journal of Antimicrobial Agents, 2020, 55, 105884.	2.5	19

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91	Synthesis and anticancer activity of aminopropoxytriterpenoids. Medicinal Chemistry Research, 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. Planta Medica, 2015, 81, 495-506.	1.3	18
93	Synthesis and chemoinformatics analysis of N-aryl-Î²-alanine derivatives. Research on Chemical Intermediates, 2015, 41, 7517-7540.	2.7	18
94	Web Resources for Discovery and Development of New Medicines. Pharmaceutical Chemistry Journal, 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. International Journal of Molecular Sciences, 2018, 19, 2519.	4.1	18
96	HIV Resistance Prediction to Reverse Transcriptase Inhibitors: Focus on Open Data. Molecules, 2018, 23, 956.	3.8	18
97	Novel antimicrobial agentsâ€™ discovery among the steroid derivatives. Steroids, 2019, 144, 52-65.	1.8	18
98	New Caffeic Acid Derivatives as Antimicrobial Agents: Design, Synthesis, Evaluation and Docking. Current Topics in Medicinal Chemistry, 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. SAR and QSAR in Environmental Research, 2002, 13, 457-471.	2.2	17
100	Why relevant chemical information cannot be exchanged without disclosing structures. Journal of Computer-Aided Molecular Design, 2005, 19, 705-713.	2.9	17
101	Prediction of biological activity profiles of cyanobacterial secondary metabolites. SAR and QSAR in Environmental Research, 2007, 18, 629-643.	2.2	17
102	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. PLoS ONE, 2014, 9, e100386.	2.5	17
103	Computer-aided design and discovery of proteinâ€“protein interaction inhibitors as agents for anti-HIV therapy. SAR and QSAR in Environmental Research, 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. Frontiers in Pharmacology, 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. International Journal of Molecular Sciences, 2020, 21, 7492.	4.1	17
106	The SistematX Web Portal of Natural Products: An Update. Journal of Chemical Information and Modeling, 2021, 61, 2516-2522.	5.4	17
107	Triazolo Based-Thiadiazole Derivatives. Synthesis, Biological Evaluation and Molecular Docking Studies. Antibiotics, 2021, 10, 804.	3.7	17
108	CYCLONET--an integrated database on cell cycle regulation and carcinogenesis. Nucleic Acids Research, 2007, 35, D550-D556.	14.5	16

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109	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. Pharmaceutical Chemistry Journal, 2017, 50, 775-780.	0.8	16
110	Pharmacological repositioning of Achyranthes aspera as an antidepressant using pharmacoinformatic tools PASS and PharmaExpert: a case study with wet lab validation. SAR and QSAR in Environmental Research, 2018, 29, 69-81.	2.2	16
111	Data Mining Approach for Extraction of Useful Information About Biologically Active Compounds from Publications. Journal of Chemical Information and Modeling, 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. Pharmaceuticals, 2020, 13, 229.	3.8	16
113	Computer Design of Vaccines: Approaches, Software Tools and Informational Resources. Current Computer-Aided Drug Design, 2005, 1, 207-222.	1.2	15
114	PASS-based approach to predict HIV-1 reverse transcriptase resistance. Journal of Bioinformatics and Computational Biology, 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. Journal of Biomedical Informatics, 2018, 85, 114-125.	4.3	15
116	Naturally occurring of Î±,Î²-diepoxy-containing compounds: origin, structures, and biological activities. Applied Microbiology and Biotechnology, 2019, 103, 3249-3264.	3.6	15
117	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. Molecules, 2019, 24, 3955.	3.8	15
118	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. Molecular Informatics, 2020, 39, e2000093.	2.5	15
119	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. Current Topics in Medicinal Chemistry, 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. BMC Bioinformatics, 2010, 11, 313.	2.6	14
121	Identification of Drug-Induced Myocardial Infarction-Related Protein Targets through the Prediction of Drugâ€“Target Interactions and Analysis of Biological Processes. Chemical Research in Toxicology, 2014, 27, 1263-1281.	3.3	14
122	Novel HIV-1 Integrase Inhibitor Development by Virtual Screening Based on QSAR Models. Current Topics in Medicinal Chemistry, 2015, 16, 441-448.	2.1	14
123	Antiprotozoal and Antitumor Activity of Natural Polycyclic Endoperoxides: Origin, Structures and Biological Activity. Molecules, 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. Pharmaceutical Chemistry Journal, 1998, 32, 658-664.	0.8	13
126	Metatox - Web application for generation of metabolic pathways and toxicity estimation. Journal of Bioinformatics and Computational Biology, 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. International Journal of Molecular Sciences, 2020, 21, 748.	4.1	13
128	Endocrine disruption profile analysis of 11,416 chemicals from chemometrical toolsâŠ¥. SAR and QSAR in Environmental Research, 2007, 18, 181-193.	2.2	12
129	In silicomethod for identification of promising anticancer drug targets. SAR and QSAR in Environmental Research, 2009, 20, 755-766.	2.2	12
130	Computer Evaluation of Drug Interactions with P-Glycoprotein. Bulletin of Experimental Biology and Medicine, 2013, 154, 521-524.	0.8	12
131	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. Molecular Informatics, 2017, 36, 1600142.	2.5	12
132	Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in Environmental Research, 2017, 28, 833-842.	2.2	12
133	Naturally occurring marine Î±,Î²-epoxy steroids: Origin and biological activities. Vietnam Journal of Chemistry, 2018, 56, 409-433.	0.8	12
134	Computer-Aided Drug Design: from Discovery of Novel Pharmaceutical Agents to Systems Pharmacology. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2020, 14, 216-227.	0.4	12
135	Antimicrobial Activity of Nitrogen-Containing 5-Î±-Androstane Derivatives: In Silico and Experimental Studies. Antibiotics, 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. Molecules, 2020, 25, 2944.	3.8	12
137	Molecular descriptor analysis of approved drugs using unsupervised learning for drug repurposing. Computers in Biology and Medicine, 2021, 138, 104856.	7.0	12
138	Computer-aided prediction of prodrug activity using the pass system. Pharmaceutical Chemistry Journal, 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. Pharmaceutical Chemistry Journal, 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. Toxicological Sciences, 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 Environmental Research, 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 Environmental Research, 2003, 14, 485-495.	2.2	10
143	Acetylenic Aquatic Anticancer Agents and Related Compounds. Natural Product Communications, 2006, 1, 1934578X0600100.	0.5	10
144	Quantum chemical simulation of cytochrome P450 catalyzed aromatic oxidation: Metabolism, toxicity, and biodegradation of benzene derivatives. International Journal of Quantum Chemistry, 2007, 107, 2454-2478.	2.0	10

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145	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. Pharmaceutical Chemistry Journal, 2012, 45, 605-611.	0.8	10
146	Identification of potential drug targets for treatment of refractory epilepsy using network pharmacology. Journal of Bioinformatics and Computational Biology, 2018, 16, 1840002.	0.8	10
147	PASS-based prediction of metabolites detection in biological systems. SAR and QSAR in Environmental Research, 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. Pharmaceutical Chemistry Journal, 2020, 53, 905-913.	0.8	10
149	Prediction of Protein Functional Specificity without an Alignment. OMICS A Journal of Integrative Biology, 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. SAR and QSAR in Environmental Research, 2015, 26, 595-604.	2.2	9
151	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. Bioinformatics, 2020, 36, 978-979.	4.1	9
152	Using systems medicine to identify a therapeutic agent with potential for repurposing in inflammatory bowel disease. DMM Disease Models and Mechanisms, 2020, 13, .	2.4	9
153	In Silico Prediction of Drugâ€“Drug Interactions Mediated by Cytochrome P450 Isoforms. Pharmaceutics, 2021, 13, 538.	4.5	9
154	Phytochemical Analysis of Polyphenol Secondary Metabolites in Cloudberry (Rubus Chamaemorus L.) Leaves. Pharmaceutical Chemistry Journal, 2021, 55, 253-258.	0.8	9
155	RECOGNITION OF PROTEIN FUNCTION USING THE LOCAL SIMILARITY. Journal of Bioinformatics and Computational Biology, 2008, 06, 709-725.	0.8	8
156	Anti-HIV Agents: Current Status and Recent Trends. Topics in Medicinal Chemistry, 2016, , 37-95.	0.8	8
157	QNA-Based Prediction of Sites of Metabolism. Molecules, 2017, 22, 2123.	3.8	8
158	Integral estimation of xenobioticsâ€™ toxicity with regard to their metabolism in human organism. Pure and Applied Chemistry, 2017, 89, 1449-1458.	1.9	8
159	Chlorinated Plant Steroids and their Biological Activities. International Journal of Current Research in Biosciences and Plant Biology, 2017, 4, 70-85.	0.1	8
160	Pharmacological Activities of Epithio Steroids. Journal of Pharmaceutical Research International, 2017, 18, 1-19.	1.0	8
161	Computer-aided prediction of receptor profile for drug-like compounds. SAR and QSAR in Environmental Research, 2002, 13, 433-444.	2.2	7
162	Internet System Predicting the Spectrum of Biological Activity of Chemical Compounds. Pharmaceutical Chemistry Journal, 2002, 36, 538-543.	0.8	7

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163	In Silico fragment-based drug design using a PASS approach. SAR and QSAR in Environmental Research, 2012, 23, 279-296.	2.2	7
164	Computer modeling of blood brain barrier permeability for physiologically active compounds. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2013, 7, 95-107.	0.4	7
165	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.	3.2	7
166	Extraction of Data on Parent Compounds and Their Metabolites from Texts of Scientific Abstracts. Journal of Chemical Information and Modeling, 2021, 61, 1683-1690.	5.4	7
167	Chromenol Derivatives as Novel Antifungal Agents: Synthesis, In Silico and In Vitro Evaluation. Molecules, 2021, 26, 4304.	3.8	7
168	About Factors Providing the Fast Protein-Protein Recognition in Processes of Complex Formation. Journal of Biomolecular Structure and Dynamics, 2003, 21, 257-266.	3.5	6
169	Synthesis and anti-inflammatory activity of ethynylthiazoles. Chemistry of Heterocyclic Compounds, 2006, 42, 675-680.	1.2	6
170	Prediction of protein post-translational modifications: main trends and methods. Russian Chemical Reviews, 2014, 83, 143-154.	6.5	6
171	Drug Repositioning: New Opportunities for Older Drugs. , 2019, , 3-17.		6
172	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. Molecules, 2020, 25, 87.	3.8	6
173	Prediction of Proteinâ€“ligand Interaction Based on Sequence Similarity and Ligand Structural Features. International Journal of Molecular Sciences, 2020, 21, 8152.	4.1	6
174	COVID-19: Analysis of Drug Repositioning Practice. Pharmaceutical Chemistry Journal, 2021, 54, 989-996.	0.8	6
175	Antitumor Profile of Carbon-Bridged Steroids (CBS) and Triterpenoids. Marine Drugs, 2021, 19, 324.	4.6	6
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