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	HIV-1 drug resistance profiling using amino acid sequence space cartography. Bioinformatics, 2022, 38, 2307-2314.	4.1	5
2	Synthesis, Biological Evaluation and Molecular Docking Studies of 5-Indolylmethylen-4-oxo-2-thioxothiazolidine Derivatives. Molecules, 2022, 27, 1068.	3.8	6
3	Relationships between the Structure and Severe Drug-Induced Liver Injury for Low, Medium, and High Doses of Drugs. Chemical Research in Toxicology, 2022, 35, 402-411.	3.3	4
4	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain. Computational Biology and Chemistry, 2022, 98, 107674.	2.3	4
5	A Potential Method for Standardization of Multiphytoadaptogen: Tandem Mass Spectrometry for Analysis of Biologically Active Substances from Rhodiola rosea. Pharmaceutical Chemistry Journal, 2022, 56, 78-84.	0.8	6
6	Computer-aided discovery of pleiotropic effects: Anti-inflammatory action of dithioloquinolinethiones as a case study. SAR and QSAR in Environmental Research, 2022, 33, 273-287.	2.2	3
7	Novel mitochondria-targeting compounds selectively kill human leukemia cells. Leukemia, 2022, 36, 2009-2021.	7.2	4
8	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. Molecular Informatics, 2021, 40, 2000231.	2.5	5
9	Antiprotozoal and Antitumor Activity of Natural Polycyclic Endoperoxides: Origin, Structures and Biological Activity. Molecules, 2021, 26, 686.	3.8	14
10	COVID-19: Analysis of Drug Repositioning Practice. Pharmaceutical Chemistry Journal, 2021, 54, 989-996.	0.8	6
11	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
12	In Silico Prediction of Drugâ€“Drug Interactions Mediated by Cytochrome P450 Isoforms. Pharmaceutics, 2021, 13, 538.	4.5	9
13	Machine Learning in Discovery of New Antivirals and Optimization of Viral Infections Therapy. Current Medicinal Chemistry, 2021, 28, .	2.4	4
14	The SistematX Web Portal of Natural Products: An Update. Journal of Chemical Information and Modeling, 2021, 61, 2516-2522.	5.4	17
15	Phytochemical Analysis of Polyphenol Secondary Metabolites in Cloudberry (Rubus Chamaemorus L.) Leaves. Pharmaceutical Chemistry Journal, 2021, 55, 253-258.	0.8	9
16	RHIVDB: A Freely Accessible Database of HIV Amino Acid Sequences and Clinical Data of Infected Patients. Frontiers in Genetics, 2021, 12, 679029.	2.3	4
17	Antitumor Profile of Carbon-Bridged Steroids (CBS) and Triterpenoids. Marine Drugs, 2021, 19, 324.	4.6	6
18	Chromenol Derivatives as Novel Antifungal Agents: Synthesis, In Silico and In Vitro Evaluation. Molecules, 2021, 26, 4304.	3.8	7

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19	Triazolo Based-Thiadiazole Derivatives. Synthesis, Biological Evaluation and Molecular Docking Studies. Antibiotics, 2021, 10, 804.	3.7	17
20	Molecular descriptor analysis of approved drugs using unsupervised learning for drug repurposing. Computers in Biology and Medicine, 2021, 138, 104856.	7.0	12
21	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
22	Possibilities of in Silico Estimations for the Development of the Pharmaceutical Composition Phytoladaptogene Cytotoxic for Bladder Cancer Cells. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2021, 15, 290-300.	0.4	1
23	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. Bioinformatics, 2020, 36, 978-979.	4.1	9
24	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. Molecules, 2020, 25, 87.	3.8	6
25	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
26	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
27	Chemical Diversity of Soft Coral Steroids and Their Pharmacological Activities. Marine Drugs, 2020, 18, 613.	4.6	27
28	Prediction of Proteinâ€“ligand Interaction Based on Sequence Similarity and Ligand Structural Features. International Journal of Molecular Sciences, 2020, 21, 8152.	4.1	6
29	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
30	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
31	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
32	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
33	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
34	Automated Extraction of Information From Texts of Scientific Publications: Insights Into HIV Treatment Strategies. Frontiers in Genetics, 2020, 11, 618862.	2.3	4
35	Antimicrobial Activity of Nitrogen-Containing 5-Î±-Androstane Derivatives: In Silico and Experimental Studies. Antibiotics, 2020, 9, 224.	3.7	12
36	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

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37	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
38	Antibacterial activity of griseofulvin analogues as an example of drug repurposing. International Journal of Antimicrobial Agents, 2020, 55, 105884.	2.5	19
39	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
40	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
41	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
42	Rationale for use mefloquine for COVID-19 treatment. Kachestvennaya Klinicheskaya Praktika, 2020, , 103-105.	0.5	0
43	Current and future use of umifenovir in patients with COVID-19. Kachestvennaya Klinicheskaya Praktika, 2020, , 75-80.	0.5	1
44	Computer Assessment of the Xenobiotic Metabolites Formationâ€™s Probability in the Human Body. Biophysics (Russian Federation), 2020, 65, 1023-1029.	0.7	0
45	Automatic Recognition of Chemical Entity Mentions in Texts of Scientific Publications. Automatic Documentation and Mathematical Linguistics, 2020, 54, 306-315.	0.5	1
46	COVID-19: Ð°Ð½Ð°Ð»Ð¸Ð· Ð¿Ñ€Ð°ÐºÑ‚Ð¸Ñ€ÑƒÐµÐ¼Ñ‹Ñ… Ð¿Ñ€ÐµÐ¿Ð°Ñ€Ð°Ñ‚Ð¾Ð²		
47	Computer-Aided Xenobiotic Toxicity Prediction Taking into Account their Metabolism in the Human Body. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2019, 13, 228-236.	0.4	3
48	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
49	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
50	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
51	Drug-drug interaction prediction using PASS. SAR and QSAR in Environmental Research, 2019, 30, 655-664.	2.2	19
52	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.	2.2	2
53	PASS-based prediction of metabolites detection in biological systems. SAR and QSAR in Environmental Research, 2019, 30, 751-758.	2.2	10
54	Derivatives of Piperazines as Potential Therapeutic Agents for Alzheimerâ€™s Disease. Molecular Pharmacology, 2019, 95, 337-348.	2.3	26

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55	Drug Repositioning: New Opportunities for Older Drugs. , 2019, , 3-17.		6
56	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
57	Naturally occurring of Î±,Î²-diepoxy-containing compounds: origin, structures, and biological activities. Applied Microbiology and Biotechnology, 2019, 103, 3249-3264.	3.6	15
58	Novel antimicrobial agentsâ€™ discovery among the steroid derivatives. Steroids, 2019, 144, 52-65.	1.8	18
59	Computer-aided prediction of biological activity spectra for organic compounds: the possibilities and limitations. Russian Chemical Bulletin, 2019, 68, 2143-2154.	1.5	56
60	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. Molecules, 2019, 24, 3955.	3.8	15
61	Metatox - Web application for generation of metabolic pathways and toxicity estimation. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940001.	0.8	13
62	Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective. Current Medicinal Chemistry, 2019, 25, 5432-5463.	2.4	6
63	New Caffeic Acid Derivatives as Antimicrobial Agents: Design, Synthesis, Evaluation and Docking. Current Topics in Medicinal Chemistry, 2019, 19, 292-304.	2.1	18
64	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
65	Naturally occurring aromatic steroids and their biological activities. Applied Microbiology and Biotechnology, 2018, 102, 4663-4674.	3.6	29
66	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
67	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
68	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. Bioinformatics, 2018, 34, 710-712.	4.1	24
69	ADVERPredâ€“Web Service for Prediction of Adverse Effects of Drugs. Journal of Chemical Information and Modeling, 2018, 58, 8-11.	5.4	50
70	Computer Prediction of Adverse Drug Effects on the Cardiovascular System. Pharmaceutical Chemistry Journal, 2018, 52, 758-762.	0.8	3
71	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
72	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. Molecules, 2018, 23, 2751.	3.8	25

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73	Highly oxygenated isoprenoid lipids derived from fungi and fungal endophytes: Origin and biological activities. Steroids, 2018, 140, 114-124.	1.8	23
74	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
75	HIV Resistance Prediction to Reverse Transcriptase Inhibitors: Focus on Open Data. Molecules, 2018, 23, 956.	3.8	18
76	Molecular Docking Studies of HIV-1 Resistance to Reverse Transcriptase Inhibitors: Mini-Review. Molecules, 2018, 23, 1233.	3.8	37
77	Peroxy steroids derived from plant and fungi and their biological activities. Applied Microbiology and Biotechnology, 2018, 102, 7657-7667.	3.6	21
78	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. Frontiers in Chemistry, 2018, 6, 133.	3.6	27
79	Naturally occurring marine Î±,Î²-epoxy steroids: Origin and biological activities. Vietnam Journal of Chemistry, 2018, 56, 409-433.	0.8	12
80	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
81	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
82	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. Biomedical Chemistry Research and Methods, 2018, 1, e00004.	0.4	99
83	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
84	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
85	Web Resources for Discovery and Development of New Medicines. Pharmaceutical Chemistry Journal, 2017, 51, 91-99.	0.8	18
86	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobioticsâ€™ Metabolites. Journal of Chemical Information and Modeling, 2017, 57, 638-642.	5.4	50
87	Anticonvulsant activity and acute neurotoxic profile of Achyranthes aspera Linn.. Journal of Ethnopharmacology, 2017, 202, 97-102.	4.1	26
88	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. Pharmaceutical Chemistry Journal, 2017, 50, 775-780.	0.8	16
89	PASS-based approach to predict HIV-1 reverse transcriptase resistance. Journal of Bioinformatics and Computational Biology, 2017, 15, 1650040.	0.8	15
90	Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in Environmental Research, 2017, 28, 833-842.	2.2	12

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91	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
92	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
93	Pharmacological and Predicted Activities of Natural Azo Compounds. Natural Products and Bioprospecting, 2017, 7, 151-169.	4.3	44
94	Computational platform Way2Drug: from the prediction of biological activity to drug repurposing. Russian Chemical Bulletin, 2017, 66, 1832-1841.	1.5	60
95	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
96	QNA-Based Prediction of Sites of Metabolism. Molecules, 2017, 22, 2123.	3.8	8
97	Integral estimation of xenobioticsâ€™ toxicity with regard to their metabolism in human organism. Pure and Applied Chemistry, 2017, 89, 1449-1458.	1.9	8
98	Chlorinated Plant Steroids and their Biological Activities. International Journal of Current Research in Biosciences and Plant Biology, 2017, 4, 70-85.	0.1	8
99	Biological Activities of Nitro Steroids. Journal of Pharmaceutical Research International, 2017, 18, 1-19.	1.0	3
100	Pharmacological Activities of Epithio Steroids. Journal of Pharmaceutical Research International, 2017, 18, 1-19.	1.0	8
101	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	2
102	Computer-aided prediction of xenobiotic metabolism in the human body. Russian Chemical Reviews, 2016, 85, 854-879.	6.5	22
103	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
104	Online resources for the prediction of biological activity of organic compounds. Russian Chemical Bulletin, 2016, 65, 384-393.	1.5	22
105	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. Journal of Cheminformatics, 2016, 8, 68.	6.1	24
106	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
107	Anti-HIV Agents: Current Status and Recent Trends. Topics in Medicinal Chemistry, 2016, , 37-95.	0.8	8
108	In silico assessment of adverse drug reactions and associated mechanisms. Drug Discovery Today, 2016, 21, 58-71.	6.4	51

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109	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
110	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
111	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
112	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. Bioinformatics, 2015, 31, 2046-2048.	4.1	83
113	Synthesis and anticancer activity of aminopropoxytriterpenoids. Medicinal Chemistry Research, 2015, 24, 3423-3436.	2.4	18
114	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
115	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
116	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
117	Naturally occurring plant isoquinoline N-oxide alkaloids: Their pharmacological and SAR activities. Phytomedicine, 2015, 22, 183-202.	5.3	72
118	Synthesis and chemoinformatics analysis of N-aryl-Î²-alanine derivatives. Research on Chemical Intermediates, 2015, 41, 7517-7540.	2.7	18
119	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
120	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. PLoS ONE, 2014, 9, e100386.	2.5	17
121	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
122	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
123	Synthesis and anticancer activity of quinopimaric and maleopimaric acidsâ€™ derivatives. Bioorganic and Medicinal Chemistry, 2014, 22, 6481-6489.	3.0	36
124	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
125	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
126	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

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127	Prediction of protein post-translational modifications: main trends and methods. Russian Chemical Reviews, 2014, 83, 143-154.	6.5	6
128	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
129	Computer search for molecular mechanisms of ulcerogenic action of non-steroidal anti-inflammatory drugs. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2013, 7, 40-45.	0.4	4
130	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
131	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.	0.8	3
132	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
133	Computer Evaluation of Drug Interactions with P-Glycoprotein. Bulletin of Experimental Biology and Medicine, 2013, 154, 521-524.	0.8	12
134	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
135	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
136	Fragment-based lead design. Russian Chemical Reviews, 2012, 81, 158-174.	6.5	19
137	Quantitative Prediction of Antitarget Interaction Profiles for Chemical Compounds. Chemical Research in Toxicology, 2012, 25, 2378-2385.	3.3	70
138	In Silico fragment-based drug design using a PASS approach. SAR and QSAR in Environmental Research, 2012, 23, 279-296.	2.2	7
139	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. Pharmaceutical Chemistry Journal, 2012, 45, 605-611.	0.8	10
140	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
141	OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia. Journal of Biomedical Semantics, 2012, 3, S7.	1.6	21
142	Synthesis, antifungal activity and QSAR study of 2-arylhydroxynitroindoles. European Journal of Medicinal Chemistry, 2011, 46, 4374-4382.	5.5	30
143	PASS-assisted exploration of new therapeutic potential of natural products. Medicinal Chemistry Research, 2011, 20, 1509-1514.	2.4	134
144	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. Molecular Informatics, 2011, 30, 241-250.	2.5	278

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145	Computer-assisted search and optimization of new human immunodeficiency virus integrase inhibitors. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2010, 4, 59-67.	0.4	2
146	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
147	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	6.1	91
148	Multi-Targeted Natural Products Evaluation Based on Biological Activity Prediction with PASS. Current Pharmaceutical Design, 2010, 16, 1703-1717.	1.9	126
149	Investigation of the structure and prediction of the biological activity of 1,3-bis(3-cyano-6,6-dimethyl-) Tj ETQq1 1 0.784314 rgBT /Ov 2009, 45, 531-535.	1.2	1
150	Computerâ€Aided Prediction of Rodent Carcinogenicity by PASS and CISOCâ€PSCT. QSAR and Combinatorial Science, 2009, 28, 806-810.	1.4	43
151	Tools for prediction of xenobiotics interaction with human cytochrome P450. Chemistry Central Journal, 2009, 3, .	2.6	0
152	In silicomethod for identification of promising anticancer drug targets. SAR and QSAR in Environmental Research, 2009, 20, 755-766.	2.2	12
153	In silico assessment of acute toxicity in rodents. Toxicology Letters, 2009, 189, S264.	0.8	2
154	QNA-based â€˜Star Trackâ€™ QSAR approach. SAR and QSAR in Environmental Research, 2009, 20, 679-709.	2.2	84
155	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
156	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. Journal of Medicinal Chemistry, 2008, 51, 1601-1609.	6.4	161
157	Computer-aided prediction for medicinal chemistry via the Internet. SAR and QSAR in Environmental Research, 2008, 19, 27-38.	2.2	44
158	Computer-aided prediction of QT-prolongation. SAR and QSAR in Environmental Research, 2008, 19, 81-90.	2.2	27
159	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
160	RECOGNITION OF PROTEIN FUNCTION USING THE LOCAL SIMILARITY. Journal of Bioinformatics and Computational Biology, 2008, 06, 709-725.	0.8	8
161	Probabilistic Approaches in Activity Prediction. , 2008, , 182-216.		67
162	Cyclobutane-Containing Alkaloids: Origin, Synthesis, and Biological Activities. Open Medicinal Chemistry Journal, 2008, 2, 26-37.	2.4	121

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163	Natural Peroxy Anticancer Agents. Mini-Reviews in Medicinal Chemistry, 2007, 7, 571-589.	2.4	106
164	Prediction of biological activity profiles of cyanobacterial secondary metabolites. SAR and QSAR in Environmental Research, 2007, 18, 629-643.	2.2	17
165	CYCLONET--an integrated database on cell cycle regulation and carcinogenesis. Nucleic Acids Research, 2007, 35, D550-D556.	14.5	16
166	PASS: identification of probable targets and mechanisms of toxicity. SAR and QSAR in Environmental Research, 2007, 18, 101-110.	2.2	95
167	A new approach to QSAR modelling of acute toxicityâ€. SAR and QSAR in Environmental Research, 2007, 18, 285-298.	2.2	49
168	Endocrine disruption profile analysis of 11,416 chemicals from chemometrical toolsâŠ¥. SAR and QSAR in Environmental Research, 2007, 18, 181-193.	2.2	12
169	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
170	Quantitative structure-activity relationships of cyclin-dependent kinase 1 inhibitors. Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry, 2007, 1, 17-28.	0.4	1
171	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
172	Acetylenic Aquatic Anticancer Agents and Related Compounds. Natural Product Communications, 2006, 1, 1934578X0600100.	0.5	10
173	Synthesis and anti-inflammatory activity of ethynylthiazoles. Chemistry of Heterocyclic Compounds, 2006, 42, 675-680.	1.2	6
174	Prediction of Protein Functional Specificity without an Alignment. OMICS A Journal of Integrative Biology, 2006, 10, 56-65.	2.0	9
175	A New Statistical Approach to Predicting Aromatic Hydroxylation Sites. Comparison with Model-Based Approaches.. ChemInform, 2005, 36, no.	0.0	0
176	Why relevant chemical information cannot be exchanged without disclosing structures. Journal of Computer-Aided Molecular Design, 2005, 19, 705-713.	2.9	17
177	Novel Antitumor Agents: Marine Sponge Alkaloids, their Synthetic Analogs and Derivatives. Mini-Reviews in Medicinal Chemistry, 2005, 5, 319-336.	2.4	106
178	Computer Design of Vaccines: Approaches, Software Tools and Informational Resources. Current Computer-Aided Drug Design, 2005, 1, 207-222.	1.2	15
179	Postgenomic chemistry (IUPAC Technical Report). Pure and Applied Chemistry, 2005, 77, 1641-1654.	1.9	5
180	Computer-aided rodent carcinogenicity prediction. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2005, 586, 138-146.	1.7	21

#	Article	IF	Citations
181	Pass. , 2005, , 459-478.		14
182	Role of the Electrostatic Interactions in Pre-orientation of Subunits in the Formation of Protein-protein Complexes. Journal of Biomolecular Structure and Dynamics, 2004, 22, 111-117.	3.5	2
183	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
184	Quantitative Relationships Between Structure and Delayed Neurotoxicity of Chemicals Studied by the Self-Consistent Regression Method Using the Pass Program. Pharmaceutical Chemistry Journal, 2004, 38, 188-190.	0.8	3
185	Design, synthesis, computational and biological evaluation of new anxiolytics. Bioorganic and Medicinal Chemistry, 2004, 12, 6559-6568.	3.0	114
186	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
187	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
188	Modern Trends in Research and Development of Antiasthmatic and Antiallergic Drugs. Pharmaceutical Chemistry Journal, 2003, 37, 293-297.	0.8	2
189	What Forces Can Determine the Formation of Highly Specific Proteinâ€“Protein Complexes?. Molecular Biology, 2003, 37, 148-155.	1.3	1
190	Predicting Biotransformation Potential from Molecular Structure.. ChemInform, 2003, 34, no.	0.0	1
191	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
192	Computer-Aided Selection of Potential Antihypertensive Compounds with Dual Mechanism of Action. Journal of Medicinal Chemistry, 2003, 46, 3326-3332.	6.4	40
193	Predicting Biotransformation Potential from Molecular Structure. Journal of Chemical Information and Computer Sciences, 2003, 43, 1636-1646.	2.8	40
194	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
195	Prediction of Biological Activity Spectra via The Internet. SAR and QSAR in Environmental Research, 2003, 14, 339-347.	2.2	56
196	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
197	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
198	Computer-aided prediction of receptor profile for drug-like compounds. SAR and QSAR in Environmental Research, 2002, 13, 433-444.	2.2	7

#	Article	IF	Citations
199	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
200	Internet System Predicting the Spectrum of Biological Activity of Chemical Compounds. Pharmaceutical Chemistry Journal, 2002, 36, 538-543.	0.8	7
201	Integrase Inhibitors: Possible Future of Anti-HIV/Aids Therapy (A Review). Pharmaceutical Chemistry Journal, 2002, 36, 575-580.	0.8	1
202	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
203	Discriminating between Drugs and Nondrugs by Prediction of Activity Spectra for Substances (PASS). Journal of Medicinal Chemistry, 2001, 44, 2432-2437.	6.4	124
204	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
205	Computer-Aided Search for Potential Drugs Exhibiting a Combined Antihypertensive Effect. Pharmaceutical Chemistry Journal, 2001, 35, 375-381.	0.8	1
206	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
207	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
208	Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics. Russian Journal of Bioorganic Chemistry, 2000, 26, 297-305.	1.0	1
209	Mapping of the active site of alcohol dehydrogenase with low-molecular ligands. Russian Journal of Bioorganic Chemistry, 2000, 26, 157-163.	1.0	0
210	The synthesis and hepatoprotective activity of esters of the lupane group triterpenoids. Russian Journal of Bioorganic Chemistry, 2000, 26, 192-200.	1.0	28
211	PASS: prediction of activity spectra for biologically active substances. Bioinformatics, 2000, 16, 747-748.	4.1	737
212	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
213	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
214	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
215	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
216	Computer-Aided Estimation of Synthetic CompoundsSimilarity with Endogenous Bioregulations. QSAR and Combinatorial Science, 1998, 17, 459-464.	1.2	6

#	Article	IF	Citations
217	Computer-aided prediction of prodrug activity using the pass system. Pharmaceutical Chemistry Journal, 1996, 30, 760-763.	0.8	11
218	Optimization of the synthesis and pharmacological characterization of substances on the basis of computer aided prognosis of biological activity spectra. Pharmaceutical Chemistry Journal, 1996, 30, 570-573.	0.8	4
219	On the creation of a russian section of the international quantitative structure â€" Activity relationship (QSAR) and modeling society. Pharmaceutical Chemistry Journal, 1996, 30, 662-663.	0.8	0
220	A possible mechanism of probucol and cholesterol interaction. Pharmaceutical Chemistry Journal, 1995, 29, 395-397.	0.8	0
221	Novel Allosteric Mechanism of P53 Activation by Small Molecules for Targeted Anticancer Therapy. SSRN Electronic Journal, 0, , .	0.4	0