V V Poroikov

List of Publications by Year in Descending Order

212 papers	5,757 citations	37 h-index	68 g-index
262 ext. papers	6,997 ext. citations	3.9 avg, IF	5.85 L-index

#	Paper	IF	Citations
212	The method predicting interaction between protein targets and small-molecular ligands with the wide applicability domain.. *Computational Biology and Chemistry*, **2022**, 98, 107674	3.6	0
211	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	0.9	1
210	Computer-aided discovery of pleiotropic effects: Anti-inflammatory action of dithioloquinolinethiones as a case study.. *SAR and QSAR in Environmental Research*, **2022**, 1-15	3.5	0
209	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	0
208	Machine Learning Methods in Antiviral Drug Discovery. *Topics in Medicinal Chemistry*, **2021**, 245-279	0.4	0
207	Extraction of Data on Parent Compounds and Their Metabolites from Texts of Scientific Abstracts. *Journal of Chemical Information and Modeling*, **2021**, 61, 1683-1690	6.1	0
206	In Silico Prediction of Drug-Drug Interactions Mediated by Cytochrome P450 Isoforms. *Pharmaceutics*, **2021**, 13,	6.4	4
205	The SistematX Web Portal of Natural Products: An Update. *Journal of Chemical Information and Modeling*, **2021**, 61, 2516-2522	6.1	3
204	Phytochemical Analysis of Polyphenol Secondary Metabolites in Cloudberry (Rubus Chamaemorus L.) Leaves. *Pharmaceutical Chemistry Journal*, **2021**, 55, 253-258	0.9	4
203	RHIVDB: A Freely Accessible Database of HIV Amino Acid Sequences and Clinical Data of Infected Patients. *Frontiers in Genetics*, **2021**, 12, 679029	4.5	2
202	Antitumor Profile of Carbon-Bridged Steroids (CBS) and Triterpenoids. *Marine Drugs*, **2021**, 19,	6	2
201	Chromenol Derivatives as Novel Antifungal Agents: Synthesis, In Silico and In Vitro Evaluation. *Molecules*, **2021**, 26,	4.8	2
200	MetaPASS: A Web Application for Analyzing the Biological Activity Spectrum of Organic Compounds Taking into Account their Biotransformation. *Molecular Informatics*, **2021**, 40, e2000231	3.8	2
199	Antiprotozoal and Antitumor Activity of Natural Polycyclic Endoperoxides: Origin, Structures and Biological Activity. *Molecules*, **2021**, 26,	4.8	4
198	COVID-19: Analysis of Drug Repositioning Practice. *Pharmaceutical Chemistry Journal*, **2021**, 54, 1-8	0.9	3
197	Triazolo Based-Thiadiazole Derivatives. Synthesis, Biological Evaluation and Molecular Docking Studies. *Antibiotics*, **2021**, 10,	4.9	9
196	Molecular descriptor analysis of approved drugs using unsupervised learning for drug repurposing. *Computers in Biology and Medicine*, **2021**, 138, 104856	7	1

195	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
194	Antimicrobial Activity of Nitrogen-Containing 5-Alpha-androstane Derivatives: In Silico and Experimental Studies. *Antibiotics*, **2020**, 9,	4.9	7
193	Data and Text Mining Help Identify Key Proteins Involved in the Molecular Mechanisms Shared by SARS-CoV-2 and HIV-1. *Molecules*, **2020**, 25,	4.8	6
192	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
191	Antibacterial activity of griseofulvin analogues as an example of drug repurposing. *International Journal of Antimicrobial Agents*, **2020**, 55, 105884	14.3	8
190	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	0.9	7
189	A Computational Approach for the Prediction of Treatment History and the Effectiveness or Failure of Antiretroviral Therapy. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	6
188	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
187	Rationale for use mefloquine for COVID-19 treatment. *Kachestvennaya Klinicheskaya Praktika*, **2020** , 103-105	0.4	
186	Current and future use of umifenovir in patients with COVID-19. *Kachestvennaya Klinicheskaya Praktika*, **2020**, 75-80	0.4	1
185	Computer Assessment of the Xenobiotic Metabolites Formation Probability in the Human Body. *Biophysics (Russian Federation)*, **2020**, 65, 1023-1029	0.7	
184	Automatic Recognition of Chemical Entity Mentions in Texts of Scientific Publications. *Automatic Documentation and Mathematical Linguistics*, **2020**, 54, 306-315	0.6	
183	Antihypoxic Action of Panax Japonicus, Tribulus Terrestris and Dioscorea Deltoidea Cell Cultures: In Silico and Animal Studies. *Molecular Informatics*, **2020**, 39, e2000093	3.8	13
182	Chemical Diversity of Soft Coral Steroids and Their Pharmacological Activities. *Marine Drugs*, **2020**, 18,	6	11
181	Prediction of Protein-ligand Interaction Based on Sequence Similarity and Ligand Structural Features. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
180	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	3.4	11
179	Computer-Aided Estimation of Biological Activity Profiles of Drug-Like Compounds Taking into Account Their Metabolism in Human Body. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
178	Using systems medicine to identify a therapeutic agent with potential for repurposing in inflammatory bowel disease. *DMM Disease Models and Mechanisms*, **2020**, 13,	4.1	3

177	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	6
176	3-Amino-5-(indol-3-yl)methylene-4-oxo-2-thioxothiazolidine Derivatives as Antimicrobial Agents: Synthesis, Computational and Biological Evaluation. *Pharmaceuticals*, **2020**, 13,	5.2	10
175	Automated Extraction of Information From Texts of Scientific Publications: Insights Into HIV Treatment Strategies. *Frontiers in Genetics*, **2020**, 11, 618862	4.5	0
174	AntiHIV-Pred: web-resource for in silico prediction of anti-HIV/AIDS activity. *Bioinformatics*, **2020**, 36, 978-979	7.2	5
173	Data Mining Approach for Extraction of Useful Information About Biologically Active Compounds from Publications. *Journal of Chemical Information and Modeling*, **2019**, 59, 3635-3644	6.1	8
172	Drug-drug interaction prediction using PASS. *SAR and QSAR in Environmental Research*, **2019**, 30, 655-664	3.5	8
171	Improving (Q)SAR predictions by examining bias in the selection of compounds for experimental testing. *SAR and QSAR in Environmental Research*, **2019**, 30, 759-773	3.5	1
170	PASS-based prediction of metabolites detection in biological systems. *SAR and QSAR in Environmental Research*, **2019**, 30, 751-758	3.5	4
169	Derivatives of Piperazines as Potential Therapeutic Agents for Alzheimer's Disease. *Molecular Pharmacology*, **2019**, 95, 337-348	4.3	15
168	Drug Repositioning: New Opportunities for Older Drugs **2019**, 3-17		4
167	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	5.1	16
166	Naturally occurring of ⊞diepoxy-containing compounds: origin, structures, and biological activities. *Applied Microbiology and Biotechnology*, **2019**, 103, 3249-3264	5.7	7
165	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	2
164	Assessment of the cardiovascular adverse effects of drug-drug interactions through a combined analysis of spontaneous reports and predicted drug-target interactions. *PLoS Computational Biology*, **2019**, 15, e1006851	5	5
163	AntiBac-Pred: A Web Application for Predicting Antibacterial Activity of Chemical Compounds. *Journal of Chemical Information and Modeling*, **2019**, 59, 4513-4518	6.1	9
162	New Caffeic Acid Derivatives as Antimicrobial Agents: Design, Synthesis, Evaluation and Docking. *Current Topics in Medicinal Chemistry*, **2019**, 19, 292-304	3	9
161	Prediction of Drug-Drug Interactions Related to Inhibition or Induction of Drug-Metabolizing Enzymes. *Current Topics in Medicinal Chemistry*, **2019**, 19, 319-336	3	12
160	(Q)SAR Models of HIV-1 Protein Inhibition by Drug-Like Compounds. *Molecules*, **2019**, 25,	4.8	2

159	Prediction of Protein-Ligand Interaction Based on the Positional Similarity Scores Derived from Amino Acid Sequences. *International Journal of Molecular Sciences*, **2019**, 21,	6.3	7
158	Novel antimicrobial agents' discovery among the steroid derivatives. *Steroids*, **2019**, 144, 52-65	2.8	11
157	Computer-aided prediction of biological activity spectra for organic compounds: the possibilities and limitations. *Russian Chemical Bulletin*, **2019**, 68, 2143-2154	1.7	27
156	Prediction of Severity of Drug-Drug Interactions Caused by Enzyme Inhibition and Activation. *Molecules*, **2019**, 24,	4.8	6
155	Metatox - Web application for generation of metabolic pathways and toxicity estimation. *Journal of Bioinformatics and Computational Biology*, **2019**, 17, 1940001	1	8
154	Naturally occurring aromatic steroids and their biological activities. *Applied Microbiology and Biotechnology*, **2018**, 102, 4663-4674	5.7	23
153	Identification of potential drug targets for treatment of refractory epilepsy using network pharmacology. *Journal of Bioinformatics and Computational Biology*, **2018**, 16, 1840002	1	7
152	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	3.5	12
151	ROSC-Pred: web-service for rodent organ-specific carcinogenicity prediction. *Bioinformatics*, **2018**, 34, 710-712	7.2	13
150	HIV Resistance Prediction to Reverse Transcriptase Inhibitors: Focus on Open Data. *Molecules*, **2018** , 23,	4.8	9
149	Molecular Docking Studies of HIV-1 Resistance to Reverse Transcriptase Inhibitors: Mini-Review. *Molecules*, **2018**, 23,	4.8	15
148	Peroxy steroids derived from plant and fungi and their biological activities. *Applied Microbiology and Biotechnology*, **2018**, 102, 7657-7667	5.7	18
147	How to Achieve Better Results Using PASS-Based Virtual Screening: Case Study for Kinase Inhibitors. *Frontiers in Chemistry*, **2018**, 6, 133	5	16
146	Naturally occurring marine ⊞epoxy steroids: Origin and biological activities. *Vietnam Journal of Chemistry*, **2018**, 56, 409-433	0.8	7
145	Molecular property diagnostic suite for diabetes mellitus (MPDS): An integrated web portal for drug discovery and drug repurposing. *Journal of Biomedical Informatics*, **2018**, 85, 114-125	10.2	6
144	CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds. *PLoS ONE*, **2018**, 13, e0191838	3.7	62
143	Computer-aided prediction of biological activity spectra for chemical compounds: opportunities and limitation. *Biomedical Chemistry Research and Methods*, **2018**, 1, e00004	0.4	63
142	Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective. *Current Medicinal Chemistry*, **2018**, 25, 5432-5463	4.3	5

141	ADVERPred-Web Service for Prediction of Adverse Effects of Drugs. *Journal of Chemical Information and Modeling*, **2018**, 58, 8-11	6.1	34
140	Computer Prediction of Adverse Drug Effects on the Cardiovascular System. *Pharmaceutical Chemistry Journal*, **2018**, 52, 758-762	0.9	2
139	Comparison of Quantitative and Qualitative (Q)SAR Models Created for the Prediction of K and IC Values of Antitarget Inhibitors. *Frontiers in Pharmacology*, **2018**, 9, 1136	5.6	9
138	A Computational Approach for the Prediction of HIV Resistance Based on Amino Acid and Nucleotide Descriptors. *Molecules*, **2018**, 23,	4.8	12
137	Highly oxygenated isoprenoid lipids derived from fungi and fungal endophytes: Origin and biological activities. *Steroids*, **2018**, 140, 114-124	2.8	16
136	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,	6.3	11
135	In Silico Identification of Proteins Associated with Drug-induced Liver Injury Based on the Prediction of Drug-target Interactions. *Molecular Informatics*, **2017**, 36, 1600142	3.8	9
134	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	3.5	15
133	Web Resources for Discovery and Development of New Medicines. *Pharmaceutical Chemistry Journal*, **2017**, 51, 91-99	0.9	15
132	MetaTox: Web Application for Predicting Structure and Toxicity of Xenobiotics' Metabolites. *Journal of Chemical Information and Modeling*, **2017**, 57, 638-642	6.1	32
131	Anticonvulsant activity and acute neurotoxic profile of Achyranthes aspera Linn. *Journal of Ethnopharmacology*, **2017**, 202, 97-102	5	20
130	Prediction and Study of Anticonvulsant Properties of Benzimidazole Derivatives. *Pharmaceutical Chemistry Journal*, **2017**, 50, 775-780	0.9	11
129	PASS-based approach to predict HIV-1 reverse transcriptase resistance. *Journal of Bioinformatics and Computational Biology*, **2017**, 15, 1650040	1	7
128	QNA-Based Prediction of Sites of Metabolism. *Molecules*, **2017**, 22,	4.8	5
127	Prediction of metabolites of epoxidation reaction in MetaTox. *SAR and QSAR in Environmental Research*, **2017**, 28, 833-842	3.5	10
126	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	3.5	13
125	How good are publicly available web services that predict bioactivity profiles for drug repurposing?. *SAR and QSAR in Environmental Research*, **2017**, 28, 843-862	3.5	32
124	Pharmacological and Predicted Activities of Natural Azo Compounds. *Natural Products and Bioprospecting*, **2017**, 7, 151-169	4.9	27

123	Computational platform Way2Drug: from the prediction of biological activity to drug repurposing. *Russian Chemical Bulletin*, **2017**, 66, 1832-1841	1.7	21
122	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	3.5	4
121	Integral estimation of xenobiotics□toxicity with regard to their metabolism in human organism. *Pure and Applied Chemistry*, **2017**, 89, 1449-1458	2.1	7
120	Chlorinated Plant Steroids and their Biological Activities. *International Journal of Current Research in Biosciences and Plant Biology*, **2017**, 4, 70-85	3.5	3
119	Biological Activities of Nitro Steroids. *Journal of Pharmaceutical Research International*, **2017**, 18, 1-19	2.5	3
118	Pharmacological Activities of Epithio Steroids. *Journal of Pharmaceutical Research International*, **2017**, 18, 1-19	2.5	7
117	Computer-aided prediction of xenobiotic metabolism in the human body. *Russian Chemical Reviews*, **2016**, 85, 854-879	6.8	17
116	Multi-omics "upstream analysis" of regulatory genomic regions helps identifying targets against methotrexate resistance of colon cancer. *EuPA Open Proteomics*, **2016**, 13, 1-13	0.1	24
115	Online resources for the prediction of biological activity of organic compounds. *Russian Chemical Bulletin*, **2016**, 65, 384-393	1.7	16
114	Prediction of reacting atoms for the major biotransformation reactions of organic xenobiotics. *Journal of Cheminformatics*, **2016**, 8, 68	8.6	19
113	QSAR Modeling and Prediction of Drug-Drug Interactions. *Molecular Pharmaceutics*, **2016**, 13, 545-56	5.6	37
112	Anti-HIV Agents: Current Status and Recent Trends. *Topics in Medicinal Chemistry*, **2016**, 37-95	0.4	6
111	In silico assessment of adverse drug reactions and associated mechanisms. *Drug Discovery Today*, **2016**, 21, 58-71	8.8	34
110	Novel HIV-1 Integrase Inhibitor Development by Virtual Screening Based on QSAR Models. *Current Topics in Medicinal Chemistry*, **2016**, 16, 441-8	3	11
109	Capacities of computer evaluation of hidden potential of phytochemicals of medicinal plants of the traditional Indian Ayurvedic medicine. *Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry*, **2016**, 10, 43-54	0.4	1
108	Synthesis and anticancer activity of aminopropoxytriterpenoids. *Medicinal Chemistry Research*, **2015**, 24, 3423-3436	2.2	14
107	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	3.1	15
106	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	3.5	9

105	PASS Targets: Ligand-based multi-target computational system based on a public data and naïve Bayes approach. *SAR and QSAR in Environmental Research*, **2015**, 26, 783-93	3.5	32
104	Naturally occurring plant isoquinoline N-oxide alkaloids: their pharmacological and SAR activities. *Phytomedicine*, **2015**, 22, 183-202	6.5	51
103	Synthesis and chemoinformatics analysis of N-aryl-β-alanine derivatives. *Research on Chemical Intermediates*, **2015**, 41, 7517-7540	2.8	11
102	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. *Journal of Chemical Information and Modeling*, **2015**, 55, 1388-99	6.1	26
101	Identification of drug targets related to the induction of ventricular tachyarrhythmia through a systems chemical biology approach. *Toxicological Sciences*, **2015**, 145, 321-36	4.4	8
100	SOMP: web server for in silico prediction of sites of metabolism for drug-like compounds. *Bioinformatics*, **2015**, 31, 2046-8	7.2	55
99	Metabolism site prediction based on xenobiotic structural formulas and PASS prediction algorithm. *Journal of Chemical Information and Modeling*, **2014**, 54, 498-507	6.1	42
98	Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. *Chemistry of Heterocyclic Compounds*, **2014**, 50, 444-457	1.4	340
97	Synthesis and anticancer activity of quinopimaric and maleopimaric acids' derivatives. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 6481-9	3.4	25
96	Chemo- and bioinformatics resources for in silico drug discovery from medicinal plants beyond their traditional use: a critical review. *Natural Product Reports*, **2014**, 31, 1585-611	15.1	85
95	Identification of drug-induced myocardial infarction-related protein targets through the prediction of drug-target interactions and analysis of biological processes. *Chemical Research in Toxicology*, **2014**, 27, 1263-81	4	11
94	Computer-aided design and discovery of protein-protein interaction inhibitors as agents for anti-HIV therapy. *SAR and QSAR in Environmental Research*, **2014**, 25, 457-71	3.5	10
93	Prediction of protein post-translational modifications: main trends and methods. *Russian Chemical Reviews*, **2014**, 83, 143-154	6.8	6
92	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	23
91	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	0.9	9
90	Design, synthesis and pharmacological evaluation of novel vanadium-containing complexes as antidiabetic agents. *PLoS ONE*, **2014**, 9, e100386	3.7	16
89	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
88	DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula. *Bioinformatics*, **2013**, 29, 2062-3	7.2	55

87	Virtual Screening for Potential Substances for the Prophylaxis of HIV Infection in Libraries of Commercially Available Organic Compounds. *Pharmaceutical Chemistry Journal*, **2013**, 47, 343-360	0.9	3
86	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	5.3	81
85	Computer evaluation of drug interactions with P-glycoprotein. *Bulletin of Experimental Biology and Medicine*, **2013**, 154, 521-4	0.8	9
84	Computer modeling of blood brain barrier permeability for physiologically active compounds. *Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry*, **2013**, 7, 95-107	0.4	5
83	Structural-Functional Analysis of 2,1,3-Benzoxadiazoles and Their N-oxides As HIV-1 Integrase Inhibitors. *Acta Naturae*, **2013**, 5, 63-72	2.1	17
82	Fragment-based design, docking, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors. *European Journal of Medicinal Chemistry*, **2012**, 47, 111-24	6.8	61
81	OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia. *Journal of Biomedical Semantics*, **2012**, 3 Suppl 1, S7	2.2	18
80	Fragment-based lead design. *Russian Chemical Reviews*, **2012**, 81, 158-174	6.8	16
79	Quantitative prediction of antitarget interaction profiles for chemical compounds. *Chemical Research in Toxicology*, **2012**, 25, 2378-85	4	50
78	In silico fragment-based drug design using a PASS approach. *SAR and QSAR in Environmental Research*, **2012**, 23, 279-96	3.5	4
77	Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. *Pharmaceutical Chemistry Journal*, **2012**, 45, 605-611	0.9	10
76	Synthesis, antifungal activity and QSAR study of 2-arylhydroxynitroindoles. *European Journal of Medicinal Chemistry*, **2011**, 46, 4374-82	6.8	29
75	PASS-assisted exploration of new therapeutic potential of natural products. *Medicinal Chemistry Research*, **2011**, 20, 1509-1514	2.2	90
74	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. *Molecular Informatics*, **2011**, 30, 241-50	3.8	172
73	Multi-targeted natural products evaluation based on biological activity prediction with PASS. *Current Pharmaceutical Design*, **2010**, 16, 1703-17	3.3	99
72	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	1
71	Functional classification of proteins based on projection of amino acid sequences: application for prediction of protein kinase substrates. *BMC Bioinformatics*, **2010**, 11, 313	3.6	13
70	Collaborative development of predictive toxicology applications. *Journal of Cheminformatics*, **2010**, 2, 7	8.6	76

69	Investigation of the structure and prediction of the biological activity of 1,3-bis(3-cyano-6,6-dimethyl- 2-oxo-5,6-dihydro-2H-pyran-4-yl)- 2-(4-methoxyphenyl)propane*. *Chemistry of Heterocyclic Compounds*, **2009**, 45, 531-535	1.4	1
68	Computer-Aided Prediction of Rodent Carcinogenicity by PASS and CISOC-PSCT. *QSAR and Combinatorial Science*, **2009**, 28, 806-810		38
67	In silico method for identification of promising anticancer drug targets. *SAR and QSAR in Environmental Research*, **2009**, 20, 755-66	3.5	8
66	QNA-based 'Star Track' QSAR approach. *SAR and QSAR in Environmental Research*, **2009**, 20, 679-709	3.5	58
65	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, 473-81	6.8	35
64	Computer-aided prediction for medicinal chemistry via the Internet. *SAR and QSAR in Environmental Research*, **2008**, 19, 27-38	3.5	36
63	Computer-aided prediction of QT-prolongation. *SAR and QSAR in Environmental Research*, **2008**, 19, 81-90	3.5	17
62	Directions in QSAR modeling for regulatory uses in OECD member countries, EU and in Russia. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2008**, 26, 201-36	4.5	29
61	Recognition of protein function using the local similarity. *Journal of Bioinformatics and Computational Biology*, **2008**, 6, 709-25	1	6
60	Chapter 6:Probabilistic Approaches in Activity Prediction **2008**, 182-216		49
59	Cyclobutane-containing alkaloids: origin, synthesis, and biological activities. *Open Medicinal Chemistry Journal*, **2008**, 2, 26-37	1.2	102
58	Computer-aided discovery of anti-inflammatory thiazolidinones with dual cyclooxygenase/lipoxygenase inhibition. *Journal of Medicinal Chemistry*, **2008**, 51, 1601-9	8.3	136
57	Endocrine disruption profile analysis of 11,416 chemicals from chemometrical tools. *SAR and QSAR in Environmental Research*, **2007**, 18, 181-93	3.5	11
56	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	2.1	8
55	Quantitative structure-activity relationships of cyclin-dependent kinase 1 inhibitors. *Biochemistry (Moscow) Supplement Series B: Biomedical Chemistry*, **2007**, 1, 17-28	0.4	1
54	Natural peroxy anticancer agents. *Mini-Reviews in Medicinal Chemistry*, **2007**, 7, 571-89	3.2	93
53	Prediction of biological activity profiles of cyanobacterial secondary metabolites. *SAR and QSAR in Environmental Research*, **2007**, 18, 629-43	3.5	16
52	CYCLONET--an integrated database on cell cycle regulation and carcinogenesis. *Nucleic Acids Research*, **2007**, 35, D550-6	20.1	13

51	PASS: identification of probable targets and mechanisms of toxicity. *SAR and QSAR in Environmental Research*, **2007**, 18, 101-10	3.5	71
50	A new approach to QSAR modelling of acute toxicity. *SAR and QSAR in Environmental Research*, **2007**, 18, 285-98	3.5	39
49	Prediction of protein functional specificity without an alignment. *OMICS A Journal of Integrative Biology*, **2006**, 10, 56-65	3.8	7
48	Rational design of macrolides by virtual screening of combinatorial libraries generated through in silico manipulation of polyketide synthases. *Journal of Medicinal Chemistry*, **2006**, 49, 2077-87	8.3	25
47	Acetylenic Aquatic Anticancer Agents and Related Compounds. *Natural Product Communications*, **2006**, 1, 1934578X0600100	0.9	3
46	Synthesis and anti-inflammatory activity of ethynylthiazoles. *Chemistry of Heterocyclic Compounds*, **2006**, 42, 675-680	1.4	4
45	Postgenomic chemistry (IUPAC Technical Report). *Pure and Applied Chemistry*, **2005**, 77, 1641-1654	2.1	5
44	Computer-aided rodent carcinogenicity prediction. *Mutation Research - Genetic Toxicology and Environmental Mutagenesis*, **2005**, 586, 138-46	3	18
43	Why relevant chemical information cannot be exchanged without disclosing structures. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 705-13	4.2	13
42	Novel antitumor agents: marine sponge alkaloids, their synthetic analogs and derivatives. *Mini-Reviews in Medicinal Chemistry*, **2005**, 5, 319-36	3.2	95
41	Computer Design of Vaccines: Approaches, Software Tools and Informational Resources. *Current Computer-Aided Drug Design*, **2005**, 1, 207-222	1.4	12
40	Pass **2005**, 459-478		12
39	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, 111-8	3.6	2
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