Igor V Tetko

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/5676436/publications.pdf

Version: 2024-02-01

191 papers	14,103 citations	31976 53 h-index	20961 115 g-index
202 all docs	202 docs citations	202 times ranked	14300 citing authors

#	Article	IF	Citations
1	Virtual Computational Chemistry Laboratory â€“ Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	2.9	1,250
2	The FunCat, a functional annotation scheme for systematic classification of proteins from whole genomes. Nucleic Acids Research, 2004, 32, 5539-5545.	14.5	988
3	The Fusarium graminearum Genome Reveals a Link Between Localized Polymorphism and Pathogen Specialization. Science, 2007, 317, 1400-1402.	12.6	837
4	Neural network studies. 1. Comparison of overfitting and overtraining. Journal of Chemical Information and Computer Sciences, 1995, 35, 826-833.	2.8	570
5	Application of Associative Neural Networks for Prediction of Lipophilicity in ALOGPS 2.1 Program. Journal of Chemical Information and Computer Sciences, 2002, 42, 1136-1145.	2.8	523
6	Calculation of Molecular Lipophilicity: State-of-the-Art and Comparison of LogP Methods on more than 96,000 Compounds. Journal of Pharmaceutical Sciences, 2009, 98, 861-893.	3.3	517
7	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	2.9	453
8	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
9	Prediction ofn-Octanol/Water Partition Coefficients from PHYSPROP Database Using Artificial Neural Networks and E-State Indices. Journal of Chemical Information and Computer Sciences, 2001, 41, 1407-1421.	2.8	360
10	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
11	Gene selection from microarray data for cancer classificationâ€”a machine learning approach. Computational Biology and Chemistry, 2005, 29, 37-46.	2.3	336
12	Estimation of Aqueous Solubility of Chemical Compounds Using E-State Indices. Journal of Chemical Information and Computer Sciences, 2001, 41, 1488-1493.	2.8	319
13	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
14	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
15	Can we estimate the accuracy of ADMEâ€“Tox predictions?. Drug Discovery Today, 2006, 11, 700-707.	6.4	242
16	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	5.4	202
17	ToxAlerts: A Web Server of Structural Alerts for Toxic Chemicals and Compounds with Potential Adverse Reactions. Journal of Chemical Information and Modeling, 2012, 52, 2310-2316.	5.4	197
18	Computing chemistry on the web. Drug Discovery Today, 2005, 10, 1497-1500.	6.4	193

#	Article	IF	Citations
19	A renaissance of neural networks in drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 785-795.	5.0	182
20	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
21	Application of ALOGPS to predict 1â€octanol/water distribution coefficients, logP, and logD, of AstraZeneca inâ€house database. Journal of Pharmaceutical Sciences, 2004, 93, 3103-3110.	3.3	171
22	State-of-the-art augmented NLP transformer models for direct and single-step retrosynthesis. Nature Communications, 2020, 11, 5575.	12.8	171
23	In Silico Approaches to Prediction of Aqueous and DMSO Solubility of Drug-Like Compounds: Trends, Problems and Solutions. Current Medicinal Chemistry, 2006, 13, 223-241.	2.4	159
24	Parvalbumin deficiency affects network properties resulting in increased susceptibility to epileptic seizures. Molecular and Cellular Neurosciences, 2004, 25, 650-663.	2.2	149
25	Neural Network Studies. 2. Variable Selection. Journal of Chemical Information and Computer Sciences, 1996, 36, 794-803.	2.8	146
26	Neural Network Studies. 4. Introduction to Associative Neural Networks. Journal of Chemical Information and Computer Sciences, 2002, 42, 717-728.	2.8	146
27	Transformer-CNN: Swiss knife for QSAR modeling and interpretation. Journal of Cheminformatics, 2020, 12, 17.	6.1	134
28	Exhaustive QSPR Studies of a Large Diverse Set of Ionic Liquids:â€‰ How Accurately Can We Predict Melting Points?. Journal of Chemical Information and Modeling, 2007, 47, 1111-1122.	5.4	129
29	Application of ALOGPS 2.1 to Predict logÂDDistribution Coefficient for Pfizer Proprietary Compounds. Journal of Medicinal Chemistry, 2004, 47, 5601-5604.	6.4	123
30	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
31	Spatiotemporal activity patterns of rat cortical neurons predict responses in a conditioned task. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 1106-1111.	7.1	112
32	Neural Network Modeling for Estimation of Partition Coefficient Based on Atom-Type Electrotopological State Indices. Journal of Chemical Information and Computer Sciences, 2000, 40, 947-955.	2.8	111
33	Applications of neural networks in structure-activity relationships of a small number of molecules. Journal of Medicinal Chemistry, 1993, 36, 811-814.	6.4	88
34	BIGCHEM: Challenges and Opportunities for Big Data Analysis in Chemistry. Molecular Informatics, 2016, 35, 615-621.	2.5	85
35	Applicability domain for in silico models to achieve accuracy of experimental measurements. Journal of Chemometrics, 2010, 24, 202-208.	1.3	80
36	Identification of Small-Molecule Frequent Hitters from AlphaScreen High-Throughput Screens. Journal of Biomolecular Screening, 2014, 19, 715-726.	2.6	77

#	Article	IF	Citations
37	Internet Software for the Calculation of the Lipophilicity and Aqueous Solubility of Chemical Compounds. Journal of Chemical Information and Computer Sciences, 2001, 41, 246-252.	2.8	74
38	Associative Neural Network. Neural Processing Letters, 2002, 16, 187-199.	3.2	72
39	Inductive Transfer of Knowledge: Application of Multi-Task Learning and Feature Net Approaches to Model Tissue-Air Partition Coefficients. Journal of Chemical Information and Modeling, 2009, 49, 133-144.	5.4	71
40	How Accurately Can We Predict the Melting Points of Drug-like Compounds?. Journal of Chemical Information and Modeling, 2014, 54, 3320-3329.	5.4	70
41	Neural Network Studies. 3. Variable Selection in the Cascade-Correlation Learning Architecture. Journal of Chemical Information and Computer Sciences, 1998, 38, 651-659.	2.8	69
42	MitoP2: An Integrative Tool for the Analysis of the Mitochondrial Proteome. Molecular Biotechnology, 2008, 40, 306-315.	2.4	69
43	Benchmarking of Linear and Nonlinear Approaches for Quantitative Structureâ^'Property Relationship Studies of Metal Complexation with Ionophores. Journal of Chemical Information and Modeling, 2006, 46, 808-819.	5.4	68
44	Optimization models for cancer classification: extracting gene interaction information from microarray expression data. Bioinformatics, 2004, 20, 644-652.	4.1	65
45	A Transformer Model for Retrosynthesis. Lecture Notes in Computer Science, 2019, , 817-830.	1.3	65
46	Calculation of lipophilicity for Pt(II) complexes: Experimental comparison of several methods. Journal of Inorganic Biochemistry, 2008, 102, 1424-1437.	3.5	64
47	Comparative Study of Multitask Toxicity Modeling on a Broad Chemical Space. Journal of Chemical Information and Modeling, 2019, 59, 1062-1072.	5.4	63
48	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
49	A review of recent advances towards the development of QSAR models for toxicity assessment of ionic liquids. Journal of Hazardous Materials, 2020, 384, 121429.	12.4	61
50	The development of models to predict melting and pyrolysis point data associated with several hundred thousand compounds mined from PATENTS. Journal of Cheminformatics, 2016, 8, 2.	6.1	60
51	Efficient Partition of Learning Data Sets for Neural Network Training. Neural Networks, 1997, 10, 1361-1374.	5.9	59
52	Prediction of Acute Aquatic Toxicity toward Daphnia Magna by using the GA-kNN Method. ATLA Alternatives To Laboratory Animals, 2014, 42, 31-41.	1.0	59
53	Prediction of partition coefficient based on atomâ€type electrotopological state indices. Journal of Pharmaceutical Sciences, 1999, 88, 229-233.	3.3	57
54	A Survey of Multiâ€task Learning Methods in Chemoinformatics. Molecular Informatics, 2019, 38, e1800108.	2.5	57

#	Article	IF	Citations
55	Consensus Modeling for HTS Assays Using In silico Descriptors Calculates the Best Balanced Accuracy in Tox21 Challenge. Frontiers in Environmental Science, 2016, 4, .	3.3	55
56	A pattern grouping algorithm for analysis of spatiotemporal patterns in neuronal spike trains. 1. Detection of repeated patterns. Journal of Neuroscience Methods, 2001, 105, 1-14.	2.5	54
57	Corticofugal modulation of functional connectivity within the auditory thalamus of rat, guinea pig and cat revealed by cooling deactivation. Journal of Neuroscience Methods, 1999, 86, 161-178.	2.5	53
58	HIV-1 Reverse Transcriptase Inhibitor Design Using Artificial Neural Networks. Journal of Medicinal Chemistry, 1994, 37, 2520-2526.	6.4	51
59	Predicting the pKa of Small Molecules. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 307-327.	1.1	50
60	Volume Learning Algorithm Artificial Neural Networks for 3D QSAR Studies. Journal of Medicinal Chemistry, 2001, 44, 2411-2420.	6.4	49
61	Development of Dimethyl Sulfoxide Solubility Models Using 163â€‰000 Molecules: Using a Domain Applicability Metric to Select More Reliable Predictions. Journal of Chemical Information and Modeling, 2013, 53, 1990-2000.	5.4	48
62	Different tonic regulation of neuronal activity in the rat dorsal raphe and medial prefrontal cortex via 5-HT1A receptors. Neuroscience Letters, 2001, 304, 129-132.	2.1	47
63	Modeling the Biodegradability of Chemical Compounds Using the Online CHEmical Modeling Environment (OCHEM). Molecular Informatics, 2014, 33, 73-85.	2.5	47
64	An unsupervised automatic method for sorting neuronal spike waveforms in awake and freely moving animals. Methods, 2003, 30, 178-187.	3.8	46
65	A comparison of different QSAR approaches to modeling CYP450 1A2 inhibition. Journal of Chemical Information and Modeling, 2011, 51, 1271-1280.	5.4	46
66	Extended Functional Groups (EFG): An Efficient Set for Chemical Characterization and Structure-Activity Relationship Studies of Chemical Compounds. Molecules, 2016, 21, 1.	3.8	46
67	Differences in locomotor behavior revealed in mice deficient for the calcium-binding proteins parvalbumin, calbindin D-28k or both. Behavioural Brain Research, 2007, 178, 250-261.	2.2	45
68	Prediction of logP for Pt(II) and Pt(IV) complexes: Comparison of statistical and quantum-chemistry based approaches. Journal of Inorganic Biochemistry, 2016, 156, 1-13.	3.5	45
69	Associative Neural Network. Methods in Molecular Biology, 2008, 458, 180-197.	0.9	44
70	Large, chemically diverse dataset of logP measurements for benchmarking studies. European Journal of Pharmaceutical Sciences, 2013, 48, 21-29.	4.0	42
71	Prediction-driven matched molecular pairs to interpret QSARs and aid the molecular optimization process. Journal of Cheminformatics, 2014, 6, 48.	6.1	42
72	Modelling the toxicity of a large set of metal and metal oxide nanoparticles using the OCHEM platform. Food and Chemical Toxicology, 2018, 112, 507-517.	3.6	42

#	Article	IF	Citations
73	Largeâ€Scale Evaluation of logâ€...P Predictors: Local Corrections May Compensate Insufficient Accuracy and Need of Experimentally Testing Every Other Compound. Chemistry and Biodiversity, 2009, 6, 1837-1844.	2.1	40
74	Modeling of non-additive mixture properties using the Online CHEmical database and Modeling environment (OCHEM). Journal of Cheminformatics, 2013, 5, 4.	6.1	39
75	A pattern grouping algorithm for analysis of spatiotemporal patterns in neuronal spike trains. 2. Application to simultaneous single unit recordings. Journal of Neuroscience Methods, 2001, 105, 15-24.	2.5	37
76	Super paramagnetic clustering of protein sequences. BMC Bioinformatics, 2005, 6, 82.	2.6	37
77	Non-linear corticoâ€“cortical interactions modulated by cholinergic afferences from the rat basal forebrain. BioSystems, 2000, 58, 219-228.	2.0	36
78	Chemical space exploration guided by deep neural networks. RSC Advances, 2019, 9, 5151-5157.	3.6	33
79	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
80	Public (Q)SAR Services, Integrated Modeling Environments, and Model Repositories on the Web: State of the Art and Perspectives for Future Development. Molecular Informatics, 2017, 36, 1600082.	2.5	32
81	Trade-off Predictivity and Explainability for Machine-Learning Powered Predictive Toxicology: An in-Depth Investigation with Tox21 Data Sets. Chemical Research in Toxicology, 2021, 34, 541-549.	3.3	31
82	Augmentation Is What You Need!. Lecture Notes in Computer Science, 2019, , 831-835.	1.3	31
83	Spatiotemporal Expression Control Correlates with Intragenic Scaffold Matrix Attachment Regions (S/MARs) in Arabidopsis thaliana. PLoS Computational Biology, 2006, 2, e21.	3.2	29
84	Accurate In Silico logâ€...P Predictions: One Can't Embrace the Unembraceable. QSAR and Combinatorial Science, 2009, 28, 845-849.	1.4	29
85	The WWW as a Tool to Obtain Molecular Parameters. Mini-Reviews in Medicinal Chemistry, 2003, 3, 809-820.	2.4	28
86	Application of a Pruning Algorithm To Optimize Artificial Neural Networks for Pharmaceutical Fingerprinting. Journal of Chemical Information and Computer Sciences, 1998, 38, 660-668.	2.8	27
87	Identifying potential endocrine disruptors among industrial chemicals and their metabolites â€“ development and evaluation of in silico tools. Chemosphere, 2015, 139, 372-378.	8.2	27
88	Polynomial Neural Network for Linear and Non-linear Model Selection in Quantitative-Structure Activity Relationship Studies on the Internet. SAR and QSAR in Environmental Research, 2000, 11, 263-280.	2.2	26
89	Electronic-Topological Investigation of theStructure - Acetylcholinesterase Inhibitor Activity Relationship in the Series of N-Benzylpiperidine Derivatives. QSAR and Combinatorial Science, 2001, 20, 31-45.	1.2	26
90	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. Journal of Cheminformatics, 2020, 12, 39.	6.1	26

#	Article	IF	Citations
91	The perspectives of computational chemistry modeling. Journal of Computer-Aided Molecular Design, 2012, 26, 135-136.	2.9	25
92	ToxCast EPA in Vitro to in Vivo Challenge: Insight into the Rank-I Model. Chemical Research in Toxicology, 2016, 29, 768-775.	3.3	25
93	Fast combinatorial methods to estimate the probability of complex temporal patterns of spikes. Biological Cybernetics, 1997, 76, 397-408.	1.3	24
94	Dynamical cell assemblies in the rat auditory cortex in a reaction-time task. BioSystems, 1998, 48, 269-277.	2.0	23
95	Support vector machines for separation of mixed plant-pathogen EST collections based on codon usage. Bioinformatics, 2005, 21, 1383-1388.	4.1	23
96	Estimation of Acid Dissociation Constants Using Graph Kernels. Molecular Informatics, 2010, 29, 731-740.	2.5	23
97	PLS-Optimal: A Stepwise D-Optimal Design Based on Latent Variables. Journal of Chemical Information and Modeling, 2012, 52, 975-983.	5.4	23
98	GEN: highly efficient SMILES explorer using autodidactic generative examination networks. Journal of Cheminformatics, 2020, 12, 22.	6.1	23
99	Does â€˜Big Dataâ€™ exist in medicinal chemistry, and if so, how can it be harnessed?. Future Medicinal Chemistry, 2016, 8, 1801-1806.	2.3	22
100	Title is missing!. Neural Processing Letters, 1997, 6, 43-50.	3.2	21
101	Lattice Model for QSAR Studies. Journal of Molecular Modeling, 2000, 6, 517-526.	1.8	21
102	Surrogate data â€“ a secure way to share corporate data. Journal of Computer-Aided Molecular Design, 2005, 19, 749-764.	2.9	21
103	Luciferase Advisor: High-Accuracy Model To Flag False Positive Hits in Luciferase HTS Assays. Journal of Chemical Information and Modeling, 2018, 58, 933-942.	5.4	19
104	Evaluation of CADASTER QSAR Models for the Aquatic Toxicity of (Benzo)triazoles and Prioritisation by Consensus Prediction. ATLA Alternatives To Laboratory Animals, 2013, 41, 49-64.	1.0	18
105	Matched Molecular Pair Analysis on Large Melting Point Datasets: A Big Data Perspective. ChemMedChem, 2018, 13, 599-606.	3.2	18
106	From Big Data to Artificial Intelligence: chemoinformatics meets new challenges. Journal of Cheminformatics, 2020, 12, 74.	6.1	17
107	Pharmaceutical Fingerprinting in Phase Space. 1. Construction of Phase Fingerprints. Analytical Chemistry, 1999, 71, 2423-2430.	6.5	16
108	Separation of sequences from hostâ€“pathogen interface using triplet nucleotide frequencies. Fungal Genetics and Biology, 2007, 44, 231-241.	2.1	16

#	Article	IF	Citations
109	Identification of Small-Molecule Frequent Hitters of Glutathione S-Transferaseâ€“Glutathione Interaction. Journal of Biomolecular Screening, 2016, 21, 596-607.	2.6	16
110	The Mouse Functional Genome Database (MfunGD): functional annotation of proteins in the light of their cellular context. Nucleic Acids Research, 2006, 34, D568-D571.	14.5	15
111	A systematic approach to infer biological relevance and biases of gene network structures. Nucleic Acids Research, 2006, 34, e6-e6.	14.5	15
112	Cross-frequency coupling in mesiotemporal EEG recordings of epileptic patients. Journal of Physiology (Paris), 2010, 104, 197-202.	2.1	15
113	QSAR models and scaffold-based analysis of non-nucleoside HIV RT inhibitors. Chemometrics and Intelligent Laboratory Systems, 2015, 148, 134-144.	3.5	15
114	Deep neural network model for highly accurate prediction of BODIPYs absorption. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120577.	3.9	15
115	Deterministic Behaviour of Short Time Series. Meccanica, 1999, 34, 145-152.	2.0	14
116	Self-organising Modelling as a Part of Simulation Process. Systems Analysis Modelling Simulation, 2003, 43, 1331-1339.	0.1	14
117	MIPS bacterial genomes functional annotation benchmark dataset. Bioinformatics, 2005, 21, 2520-2521.	4.1	13
118	Rational design of isonicotinic acid hydrazide derivatives with antitubercular activity: Machine learning, molecular docking, synthesis and biological testing. Chemical Biology and Drug Design, 2018, 92, 1272-1278.	3.2	13
119	Structureâ€“Activity Relationship in Pyrazolo[4,3-c]pyridines, First Inhibitors of PEX14â€“PEX5 Proteinâ€“Protein Interaction with Trypanocidal Activity. Journal of Medicinal Chemistry, 2020, 63, 847-879.	6.4	13
120	Beyond the â€˜bestâ€™ match: machine learning annotation of protein sequences by integration of different sources of information. Bioinformatics, 2008, 24, 621-628.	4.1	12
121	Computational Toxicology. Chemical Research in Toxicology, 2020, 33, 687-688.	3.3	12
122	<title>Spatiotemporal activity patterns detected from single cell measurements from behaving animals</title>. , 1999, 3728, 20.		10
123	Calculation of molecular lipophilicity: state of the art and comparison of methods on more than 96000 compounds. Chemistry Central Journal, 2009, 3, .	2.6	10
124	Prioritisation of Polybrominated Diphenyl Ethers (PBDEs) by Using the QSPR-THESAURUS Web Tool. ATLA Alternatives To Laboratory Animals, 2013, 41, 127-135.	1.0	10
125	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
126	Structure-Activity Relationship Modeling and Experimental Validation of the Imidazolium and Pyridinium Based Ionic Liquids as Potential Antibacterials of MDR Acinetobacter baumannii and Staphylococcus aureus. International Journal of Molecular Sciences, 2021, 22, 563.	4.1	10

#	Article	IF	Citations
127	Introduction to Special Issue: Computational Toxicology. Chemical Research in Toxicology, 2021, 34, 171-175.	3.3	10
128	Pharmaceutical Fingerprinting in Phase Space. 2. Pattern Recognition. Analytical Chemistry, 1999, 71, 2431-2439.	6.5	9
129	Volume learning algorithm significantly improved PLS model for predicting the estrogenic activity of xenoestrogens. Journal of Molecular Graphics and Modelling, 2007, 26, 591-594.	2.4	9
130	From Descriptors to Predicted Properties: Experimental Design by Using Applicability Domain Estimation. ATLA Alternatives To Laboratory Animals, 2013, 41, 33-47.	1.0	9
131	Nonlinear Dimensionality Reduction for Visualizing Toxicity Data: Distanceâ€Based Versus Topologyâ€Based Approaches. ChemMedChem, 2014, 9, 1047-1059.	3.2	9
132	An evaluation of experimental design in QSAR modelling utilizing the kâ€medoid clustering. Journal of Chemometrics, 2012, 26, 509-517.	1.3	8
133	More Is Not Always Better: Local Models Provide Accurate Predictions of Spectral Properties of Porphyrins. International Journal of Molecular Sciences, 2022, 23, 1201.	4.1	8
134	Theoretical and Experimental Studies of Phosphonium Ionic Liquids as Potential Antibacterials of MDR Acinetobacter baumannii. Antibiotics, 2022, 11, 491.	3.7	8
135	Focused Library Generator: case of Mdmx inhibitors. Journal of Computer-Aided Molecular Design, 2020, 34, 769-782.	2.9	7
136	Water envelope has a critical impact on the design of proteinâ€“protein interaction inhibitors. Chemical Communications, 2020, 56, 4360-4363.	4.1	7
137	Calculation of lipophilicity for Pt(II) complexes: experimental comparison of several methods. Chemistry Central Journal, 2008, 2, .	2.6	6
138	ROBUSTNESS IN EXPERIMENTAL DESIGN: A STUDY ON THE RELIABILITY OF SELECTION APPROACHES. Computational and Structural Biotechnology Journal, 2013, 7, e201305002.	4.1	6
139	Joint Virtual Special Issue on Computational Toxicology. Journal of Chemical Information and Modeling, 2020, 60, 1069-1071.	5.4	6
140	Simple heuristic methods for input parameters' estimation in neural networks. , 1994, , .		5
141	Evaluation of potential HIV-1 reverse transcriptase inhibitors by artificial neural networks. , 0, , .		5
142	Computer assisted neurophysiological analysis of cell assemblies activity. Neurocomputing, 2001, 38-40, 1025-1030.	5.9	5
143	Dopamine modulation of activity of cat sensorimotor cortex neurons during conditioned reflexes. Neuroscience Letters, 2002, 330, 171-174.	2.1	5
144	The effects of activation of glutamate ionotropic connections of neurons in the sensorimotor cortex in a conditioned reflex. Neuroscience and Behavioral Physiology, 2003, 33, 479-488.	0.4	5

#	Article	IF	Citations
145	In silico and in vitro studies of a number PILs as new antibacterials against MDR clinical isolate Acinetobacter baumannii. Chemical Biology and Drug Design, 2020, 95, 624-630.	3.2	5
146	Using Online Tool (iPrior) for Modeling ToxCast™ Assays Towards Prioritization of Animal Toxicity Testing. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 420-438.	1.1	5
147	Title is missing!. Neural Processing Letters, 1997, 6, 51-59.	3.2	4
148	A web portal for classification of expression data using maximal margin linear programming. Bioinformatics, 2004, 20, 3284-3285.	4.1	4
149	Dopamine modulation of glutamate metabotropic receptors in conditioned reaction of sensory motor cortex neurons of the cat. Neuroscience Letters, 2004, 356, 127-130.	2.1	4
150	Eclair--a web service for unravelling species origin of sequences sampled from mixed host interfaces. Nucleic Acids Research, 2005, 33, W724-W727.	14.5	4
151	The Prediction of Physicochemical Properties. , 0, , 240-275.		4
152	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	6.1	4
153	Anti-MRSA drug discovery by ligand-based virtual screening and biological evaluation. Bioorganic Chemistry, 2021, 114, 105042.	4.1	4
154	Variable Selection in the Cascade-Correlation Learning Architecture. , 2000, , 472-473.		4
155	Early ADME/T Predictions: Toy or Tool?. , 2008, , 240-267.		4
156	Pattern grouping algorithm and de-convolution filtering of non-stationary correlated Poisson processes. Neurocomputing, 2001, 38-40, 1709-1714.	5.9	3
157	Exploiting scale-free information from expression data for cancer classification. Computational Biology and Chemistry, 2005, 29, 288-293.	2.3	3
158	FunCat functional inference with belief propagation and feature integration. Computational Biology and Chemistry, 2008, 32, 375-377.	2.3	3
159	Experimental and Theoretical Studies in the EU FP7 Marie Curie Initial Training Network Project, Environmental ChemOinformatics (ECO). ATLA Alternatives To Laboratory Animals, 2014, 42, 7-11.	1.0	3
160	Application of Self-Organizing Neural Networks with Active Neurons for Prediction of Bioactivity of Chemical Compounds by the Analogues Search Algorithm. Journal of Automation and Information Sciences, 1999, 31, 51-58.	0.7	3
161	Internet in Drug Design and Discovery. The Open Applied Informatics Journal, 2008, 2, 18-21.	1.0	3
162	Study of the structure-activity relationship in a series of physiologically active substances with a common trend of action upon the cell signaling system. Pharmaceutical Chemistry Journal, 1996, 30, 384-390.	0.8	2

#	Article	IF	Citations
163	Computer Assisted Neurophysiology by a Distributed Java Program. Journal of Biomedical Informatics, 1998, 31, 465-475.	0.7	2
164	Classification of CYP450 1A2 inhibitors using PubChem data. Journal of Cheminformatics, 2010, 2, .	6.1	2
165	OCHEM - on-line CHEmical database & modeling environment. Journal of Cheminformatics, 2010, 2, .	6.1	2
166	In silico pK a prediction. Journal of Cheminformatics, 2012, 4, .	6.1	2
167	Exemplification of the Implementation of Alternatives to Experimental Testing in Chemical Risk Assessment â€" Case Studies from the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2013, 41, 13-17.	1.0	2
168	Application of Self-Organizing Neural Networks with Active Neurons for QSAR Studies. , 2000, , 444-445.		2
169	What Features of Ligands Are Relevant to the Opening of Cryptic Pockets in Drug Targets?. Informatics, 2022, 9, 8.	3.9	2
170	DETECTION OF DETERMINISTIC DYNAMICS IN SHORT DISCRETE TIME SERIES. , 2000, , .		1
171	NON-LINEAR COUPLING OF LOCAL FIELD POTENTIALS ACROSS CORTICAL SITES IN PARVALBUMIN-DEFICIENT MICE. , 2000, , .		1
172	Title is missing!. Pharmaceutical Chemistry Journal, 2001, 35, 78-84.	0.8	1
173	Comparison of applicability domains of QSAR models: application to the modelling of the environmental toxicity against Tetrahymena pyriformis. Chemistry Central Journal, 2008, 2, .	2.6	1
174	Applicability domain for classification problems. Journal of Cheminformatics, 2010, 2, .	6.1	1
175	Highly Accurate Filters to Flag Frequent Hitters in AlphaScreen Assays by Suggesting their Mechanism. Molecular Informatics, 2021, , 2100151.	2.5	1
176	Analysis of the deterministic behaviour of experimental series. European Physical Journal Special Topics, 1998, 08, Pr6-209-Pr6-213.	0.2	1
177	Detection of elements of structural commonality of substances with similar effects on the cell signal systems. Pharmaceutical Chemistry Journal, 1992, 26, 116-120.	0.8	0
178	Modified Hopfinger analysis of the phosphodiesterase inhibiting activity of flavonoids. Theoretical and Experimental Chemistry, 1994, 29, 45-50.	0.8	0
179	Use of topological indexes for prediction of the activity of 5-lipoxygenase inhibitors in a series of hydroxamates. Theoretical and Experimental Chemistry, 1994, 29, 84-86.	0.8	0
180	Application of topological indexes to predict immunomodulating activity of new peptides. Theoretical and Experimental Chemistry, 1997, 33, 86-89.	0.8	0

#	Article	IF	Citations
181	Virtual computational chemistry laboratory: internet tool for remote modeling and design in chemical problems. , 0, , .		0
182	Burst Recognition Algorithm Based on Symmetry Properties. , 2005, , .		0
183	Data integration and knowledge transfer: application to the tissue: air partition coefficients. Chemistry Central Journal, 2009, 3, .	2.6	0
184	Online chemical modeling environment. Chemistry Central Journal, 2009, 3, .	2.6	0
185	QSAR modeling for In vitro assays: linking ToxCastâ„¢ database to the integrated modeling framework â€œOCHEMâ€. Journal of Cheminformatics, 2012, 4, .	6.1	0
186	Computer Assisted Neurophysiology by a Distributed Java Program. , 2001, , 261-272.		0
187	Recognition of Neurons Impulses with the Use of Nonlinear Dynamic Equations. Journal of Automation and Information Sciences, 2001, 33, 10.	0.7	0
188	Recognition of Signals with Application of Nonlinear Equations of Dynamics. Journal of Automation and Information Sciences, 1999, 31, 81-87.	0.7	0
189	ROBUSTNESS IN EXPERIMENTAL DESIGN: A STUDY ON THE RELIABILITY OF SELECTION APPROACHES. Cell, 2018, 5, e201305002.	28.9	0
190	Analysis and Modelling of False Positives in GPCR Assays. Lecture Notes in Computer Science, 2019, , 764-770.	1.3	0
191	Determination of chaotic attractors in short discrete time series. , 0, , .		0