Igor V Tetko

List of Publications by Year
in descending order

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	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
2	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
3	What Features of Ligands Are Relevant to the Opening of Cryptic Pockets in Drug Targets?. Informatics, 2022, 9, 8.	3.9	2
4	Theoretical and Experimental Studies of Phosphonium Ionic Liquids as Potential Antibacterials of MDR Acinetobacter baumannii. Antibiotics, 2022, 11, 491.	3.7	8
5	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
6	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
7	Introduction to Special Issue: Computational Toxicology. Chemical Research in Toxicology, 2021, 34, 171-175.	3.3	10
8	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
9	Anti-MRSA drug discovery by ligand-based virtual screening and biological evaluation. Bioorganic Chemistry, 2021, 114, 105042.	4.1	4
10	Highly Accurate Filters to Flag Frequent Hitters in AlphaScreen Assays by Suggesting their Mechanism. Molecular Informatics, 2021, , 2100151.	2.5	1
11	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
12	Focused Library Generator: case of Mdmx inhibitors. Journal of Computer-Aided Molecular Design, 2020, 34, 769-782.	2.9	7
13	Structure–Activity Relationship in Pyrazolo[4,3-c]pyridines, First Inhibitors of PEX14–PEX5 Protein–Protein Interaction with Trypanocidal Activity. Journal of Medicinal Chemistry, 2020, 63, 847-879.	6.4	13
14	State-of-the-art augmented NLP transformer models for direct and single-step retrosynthesis. Nature Communications, 2020, 11, 5575.	12.8	171
15	From Big Data to Artificial Intelligence: chemoinformatics meets new challenges. Journal of Cheminformatics, 2020, 12, 74.	6.1	17
16	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
17	Computational Toxicology. Chemical Research in Toxicology, 2020, 33, 687-688.	3.3	12
18	Water envelope has a critical impact on the design of protein–protein interaction inhibitors. Chemical Communications, 2020, 56, 4360-4363.	4.1	7

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19	Transformer-CNN: Swiss knife for QSAR modeling and interpretation. Journal of Cheminformatics, 2020, 12, 17.	6.1	134
20	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
21	Joint Virtual Special Issue on Computational Toxicology. Journal of Chemical Information and Modeling, 2020, 60, 1069-1071.	5.4	6
22	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
23	GEN: highly efficient SMILES explorer using autodidactic generative examination networks. Journal of Cheminformatics, 2020, 12, 22.	6.1	23
24	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
25	Chemical space exploration guided by deep neural networks. RSC Advances, 2019, 9, 5151-5157.	3.6	33
26	Comparative Study of Multitask Toxicity Modeling on a Broad Chemical Space. Journal of Chemical Information and Modeling, 2019, 59, 1062-1072.	5.4	63
27	A Survey of Multi‑task Learning Methods in Chemoinformatics. Molecular Informatics, 2019, 38, e1800108.	2.5	57
28	A Transformer Model for Retrosynthesis. Lecture Notes in Computer Science, 2019, , 817-830.	1.3	65
29	Augmentation Is What You Need!. Lecture Notes in Computer Science, 2019, , 831-835.	1.3	31
30	Analysis and Modelling of False Positives in GPCR Assays. Lecture Notes in Computer Science, 2019, , 764-770.	1.3	0
31	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
32	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
33	Matched Molecular Pair Analysis on Large Melting Point Datasets: A Big Data Perspective. ChemMedChem, 2018, 13, 599-606.	3.2	18
34	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
35	ROBUSTNESS IN EXPERIMENTAL DESIGN: A STUDY ON THE RELIABILITY OF SELECTION APPROACHES. Cell, 2018, 5, e201305002.	28.9	0
36	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

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37	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
38	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
39	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
40	Identification of Small-Molecule Frequent Hitters of Glutathione S-Transferase–Glutathione Interaction. Journal of Biomolecular Screening, 2016, 21, 596-607.	2.6	16
41	ToxCast EPA <i>in Vitro</i> to <i>in Vivo</i> Challenge: Insight into the Rank-I Model. Chemical Research in Toxicology, 2016, 29, 768-775.	3.3	25
42	BIGCHEM: Challenges and Opportunities for Big Data Analysis in Chemistry. Molecular Informatics, 2016, 35, 615-621.	2.5	85
43	Does 'Big Data' exist in medicinal chemistry, and if so, how can it be harnessed?. Future Medicinal Chemistry, 2016, 8, 1801-1806.	2.3	22
44	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
45	A renaissance of neural networks in drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 785-795.	5.0	182
46	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
47	QSAR models and scaffold-based analysis of non-nucleoside HIV RT inhibitors. Chemometrics and Intelligent Laboratory Systems, 2015, 148, 134-144.	3.5	15
48	Identifying potential endocrine disruptors among industrial chemicals and their metabolites – development and evaluation of in silico tools. Chemosphere, 2015, 139, 372-378.	8.2	27
49	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
50	Prediction of Acute Aquatic Toxicity toward <i>Daphnia Magna</i> by using the GA-<i>k</i>NN Method. ATLA Alternatives To Laboratory Animals, 2014, 42, 31-41.	1.0	59
51	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
52	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
53	Identification of Small-Molecule Frequent Hitters from AlphaScreen High-Throughput Screens. Journal of Biomolecular Screening, 2014, 19, 715-726.	2.6	77
54	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

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55	Prediction-driven matched molecular pairs to interpret QSARs and aid the molecular optimization process. Journal of Cheminformatics, 2014, 6, 48.	6.1	42
56	Modeling the Biodegradability of Chemical Compounds Using the Online CHEmical Modeling Environment (OCHEM). Molecular Informatics, 2014, 33, 73-85.	2.5	47
57	Nonlinear Dimensionality Reduction for Visualizing Toxicity Data: Distanceâ€Based Versus Topologyâ€Based Approaches. ChemMedChem, 2014, 9, 1047-1059.	3.2	9
58	Modeling of non-additive mixture properties using the Online CHEmical database and Modeling environment (OCHEM). Journal of Cheminformatics, 2013, 5, 4.	6.1	39
59	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
60	Large, chemically diverse dataset of logP measurements for benchmarking studies. European Journal of Pharmaceutical Sciences, 2013, 48, 21-29.	4.0	42
61	ROBUSTNESS IN EXPERIMENTAL DESIGN: A STUDY ON THE RELIABILITY OF SELECTION APPROACHES. Computational and Structural Biotechnology Journal, 2013, 7, e201305002.	4.1	6
62	From Descriptors to Predicted Properties: Experimental Design by Using Applicability Domain Estimation. ATLA Alternatives To Laboratory Animals, 2013, 41, 33-47.	1.0	9
63	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
64	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
65	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
66	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
67	PLS-Optimal: A Stepwise D-Optimal Design Based on Latent Variables. Journal of Chemical Information and Modeling, 2012, 52, 975-983.	5.4	23
68	An evaluation of experimental design in QSAR modelling utilizing the kâ€medoid clustering. Journal of Chemometrics, 2012, 26, 509-517.	1.3	8
69	In silico pK a prediction. Journal of Cheminformatics, 2012, 4, .	6.1	2
70	QSAR modeling for In vitro assays: linking ToxCastâ„¢ database to the integrated modeling framework â€œOCHEMâ€ Journal of Cheminformatics, 2012, 4, .	6.1	0
71	The perspectives of computational chemistry modeling. Journal of Computer-Aided Molecular Design, 2012, 26, 135-136.	2.9	25
72	A comparison of different QSAR approaches to modeling CYP450 1A2 inhibition. Journal of Chemical Information and Modeling, 2011, 51, 1271-1280.	5.4	46

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73	Predicting the pKa of Small Molecules. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 307-327.	1.1	50
74	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
75	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
76	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
77	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
78	Cross-frequency coupling in mesiotemporal EEG recordings of epileptic patients. Journal of Physiology (Paris), 2010, 104, 197-202.	2.1	15
79	Applicability domain for <i>in silico</i> models to achieve accuracy of experimental measurements. Journal of Chemometrics, 2010, 24, 202-208.	1.3	80
80	Estimation of Acid Dissociation Constants Using Graph Kernels. Molecular Informatics, 2010, 29, 731-740.	2.5	23
81	Classification of CYP450 1A2 inhibitors using PubChem data. Journal of Cheminformatics, 2010, 2, .	6.1	2
82	Applicability domain for classification problems. Journal of Cheminformatics, 2010, 2, .	6.1	1
83	OCHEM - on-line CHEmical database & modeling environment. Journal of Cheminformatics, 2010, 2, .	6.1	2
84	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
85	Accurate In Silico logâ€¦<i>P</i> Predictions: One Can't Embrace the Unembraceable. QSAR and Combinatorial Science, 2009, 28, 845-849.	1.4	29
86	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
87	Data integration and knowledge transfer: application to the tissue: air partition coefficients. Chemistry Central Journal, 2009, 3, .	2.6	0
88	Online chemical modeling environment. Chemistry Central Journal, 2009, 3, .	2.6	0
89	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
90	Largeâ€ Scale Evaluation of logâ€¦<i>P</i> 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

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91	Calculation of lipophilicity for Pt(II) complexes: Experimental comparison of several methods. Journal of Inorganic Biochemistry, 2008, 102, 1424-1437.	3.5	64
92	MitoP2: An Integrative Tool for the Analysis of the Mitochondrial Proteome. Molecular Biotechnology, 2008, 40, 306-315.	2.4	69
93	Calculation of lipophilicity for Pt(II) complexes: experimental comparison of several methods. Chemistry Central Journal, 2008, 2, .	2.6	6
94	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
95	FunCat functional inference with belief propagation and feature integration. Computational Biology and Chemistry, 2008, 32, 375-377.	2.3	3
96	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
97	Critical Assessment of QSAR Models of Environmental Toxicity against <i>Tetrahymena pyriformis:</i> Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
98	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
99	Associative Neural Network. Methods in Molecular Biology, 2008, 458, 180-197.	0.9	44
100	Early ADME/T Predictions: Toy or Tool?. , 2008, , 240-267.		4
101	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
102	Internet in Drug Design and Discovery. The Open Applied Informatics Journal, 2008, 2, 18-21.	1.0	3
103	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
104	Separation of sequences from hostâ€"pathogen interface using triplet nucleotide frequencies. Fungal Genetics and Biology, 2007, 44, 231-241.	2.1	16
105	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
106	The <i>Fusarium graminearum</i> Genome Reveals a Link Between Localized Polymorphism and Pathogen Specialization. Science, 2007, 317, 1400-1402.	12.6	837
107	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
108	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

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109	Can we estimate the accuracy of ADMEâ€"Tox predictions?. Drug Discovery Today, 2006, 11, 700-707.	6.4	242
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	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
113	Spatiotemporal Expression Control Correlates with Intragenic Scaffold Matrix Attachment Regions (S/MARs) in Arabidopsis thaliana. PLoS Computational Biology, 2006, 2, e21.	3.2	29
114	Gene selection from microarray data for cancer classificationâ€"a machine learning approach. Computational Biology and Chemistry, 2005, 29, 37-46.	2.3	336
115	Exploiting scale-free information from expression data for cancer classification. Computational Biology and Chemistry, 2005, 29, 288-293.	2.3	3
116	Computing chemistry on the web. Drug Discovery Today, 2005, 10, 1497-1500.	6.4	193
117	Super paramagnetic clustering of protein sequences. BMC Bioinformatics, 2005, 6, 82.	2.6	37
118	Virtual Computational Chemistry Laboratory â€" Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	2.9	1,250
119	Surrogate data â€" a secure way to share corporate data. Journal of Computer-Aided Molecular Design, 2005, 19, 749-764.	2.9	21
120	Support vector machines for separation of mixed plant-pathogen EST collections based on codon usage. Bioinformatics, 2005, 21, 1383-1388.	4.1	23
121	MIPS bacterial genomes functional annotation benchmark dataset. Bioinformatics, 2005, 21, 2520-2521.	4.1	13
122	Burst Recognition Algorithm Based on Symmetry Properties. , 2005, , .		0
123	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
124	Optimization models for cancer classification: extracting gene interaction information from microarray expression data. Bioinformatics, 2004, 20, 644-652.	4.1	65
125	The FunCat, a functional annotation scheme for systematic classification of proteins from whole genomes. Nucleic Acids Research, 2004, 32, 5539-5545.	14.5	988
126	A web portal for classification of expression data using maximal margin linear programming. Bioinformatics, 2004, 20, 3284-3285.	4.1	4

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127	Application of ALOGPS 2.1 to Predict logÂDDistribution Coefficient for Pfizer Proprietary Compounds. Journal of Medicinal Chemistry, 2004, 47, 5601-5604.	6.4	123
128	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
129	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
130	Parvalbumin deficiency affects network properties resulting in increased susceptibility to epileptic seizures. Molecular and Cellular Neurosciences, 2004, 25, 650-663.	2.2	149
131	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
132	An unsupervised automatic method for sorting neuronal spike waveforms in awake and freely moving animals. Methods, 2003, 30, 178-187.	3.8	46
133	The WWW as a Tool to Obtain Molecular Parameters. Mini-Reviews in Medicinal Chemistry, 2003, 3, 809-820.	2.4	28
134	Self-organising Modelling as a Part of Simulation Process. Systems Analysis Modelling Simulation, 2003, 43, 1331-1339.	0.1	14
135	Neural Network Studies. 4. Introduction to Associative Neural Networks. Journal of Chemical Information and Computer Sciences, 2002, 42, 717-728.	2.8	146
136	Dopamine modulation of activity of cat sensorimotor cortex neurons during conditioned reflexes. Neuroscience Letters, 2002, 330, 171-174.	2.1	5
137	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
138	Associative Neural Network. Neural Processing Letters, 2002, 16, 187-199.	3.2	72
139	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
140	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
141	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
142	Volume Learning Algorithm Artificial Neural Networks for 3D QSAR Studies. Journal of Medicinal Chemistry, 2001, 44, 2411-2420.	6.4	49
143	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
144	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

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145	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
146	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
147	Title is missing!. Pharmaceutical Chemistry Journal, 2001, 35, 78-84.	0.8	1
148	Computer assisted neurophysiological analysis of cell assemblies activity. Neurocomputing, 2001, 38-40, 1025-1030.	5.9	5
149	Pattern grouping algorithm and de-convolution filtering of non-stationary correlated Poisson processes. Neurocomputing, 2001, 38-40, 1709-1714.	5.9	3
150	Computer Assisted Neurophysiology by a Distributed Java Program. , 2001, , 261-272.		0
151	Recognition of Neurons Impulses with the Use of Nonlinear Dynamic Equations. Journal of Automation and Information Sciences, 2001, 33, 10.	0.7	0
152	DETECTION OF DETERMINISTIC DYNAMICS IN SHORT DISCRETE TIME SERIES. , 2000, , .		1
153	NON-LINEAR COUPLING OF LOCAL FIELD POTENTIALS ACROSS CORTICAL SITES IN PARVALBUMIN-DEFICIENT MICE. , 2000, , .		1
154	Non-linear cortico–cortical interactions modulated by cholinergic afferences from the rat basal forebrain. BioSystems, 2000, 58, 219-228.	2.0	36
155	Lattice Model for QSAR Studies. Journal of Molecular Modeling, 2000, 6, 517-526.	1.8	21
156	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
157	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
158	Application of Self-Organizing Neural Networks with Active Neurons for QSAR Studies. , 2000, , 444-445.		2
159	Variable Selection in the Cascade-Correlation Learning Architecture. , 2000, , 472-473.		4
160	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
161	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
162	Prediction of partition coefficient based on atom–type electrotopological state indices. Journal of Pharmaceutical Sciences, 1999, 88, 229-233.	3.3	57

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163	Deterministic Behaviour of Short Time Series. Meccanica, 1999, 34, 145-152.	2.0	14
164	Pharmaceutical Fingerprinting in Phase Space. 2. Pattern Recognition. Analytical Chemistry, 1999, 71, 2431-2439.	6.5	9
165	Pharmaceutical Fingerprinting in Phase Space. 1. Construction of Phase Fingerprints. Analytical Chemistry, 1999, 71, 2423-2430.	6.5	16
166	<title>Spatiotemporal activity patterns detected from single cell measurements from behaving animals</title>. , 1999, 3728, 20.		10
167	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
168	Recognition of Signals with Application of Nonlinear Equations of Dynamics. Journal of Automation and Information Sciences, 1999, 31, 81-87.	0.7	0
169	Computer Assisted Neurophysiology by a Distributed Java Program. Journal of Biomedical Informatics, 1998, 31, 465-475.	0.7	2
170	Dynamical cell assemblies in the rat auditory cortex in a reaction-time task. BioSystems, 1998, 48, 269-277.	2.0	23
171	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
172	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
173	Analysis of the deterministic behaviour of experimental series. European Physical Journal Special Topics, 1998, 08, Pr6-209-Pr6-213.	0.2	1
174	Title is missing!. Neural Processing Letters, 1997, 6, 43-50.	3.2	21
175	Title is missing!. Neural Processing Letters, 1997, 6, 51-59.	3.2	4
176	Application of topological indexes to predict immunomodulating activity of new peptides. Theoretical and Experimental Chemistry, 1997, 33, 86-89.	0.8	0
177	Fast combinatorial methods to estimate the probability of complex temporal patterns of spikes. Biological Cybernetics, 1997, 76, 397-408.	1.3	24
178	Efficient Partition of Learning Data Sets for Neural Network Training. Neural Networks, 1997, 10, 1361-1374.	5.9	59
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180	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

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