Alexander Tropsha

List of Publications by Year
in descending order

238	25,164	10389 72	7348 152
papers	citations	h-index	g-index

264	264	264	18136
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Beware of q2!. Journal of Molecular Graphics and Modelling, 2002, 20, 269-276.	2.4	3,216
2	The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. QSAR and Combinatorial Science, 2003, 22, 69-77.	1.4	1,698
3	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
4	Best Practices for QSAR Model Development, Validation, and Exploitation. Molecular Informatics, 2010, 29, 476-488.	2.5	1,369
5	Deep reinforcement learning for de novo drug design. Science Advances, 2018, 4, eaap7885.	10.3	740
6	Trust, But Verify: On the Importance of Chemical Structure Curation in Cheminformatics and QSAR Modeling Research. Journal of Chemical Information and Modeling, 2010, 50, 1189-1204.	5.4	611
7	Rational selection of training and test sets for the development of validated QSAR models. Journal of Computer-Aided Molecular Design, 2003, 17, 241-253.	2.9	588
8	Chemical Basis of Interactions Between Engineered Nanoparticles and Biological Systems. Chemical Reviews, 2014, 114, 7740-7781.	47.7	478
9	Novel Variable Selection Quantitative Structureâ^'Property Relationship Approach Based on thek-Nearest-Neighbor Principle. Journal of Chemical Information and Computer Sciences, 2000, 40, 185-194.	2.8	436
10	Universal fragment descriptors for predicting properties of inorganic crystals. Nature Communications, 2017, 8, 15679.	12.8	435
11	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
12	Predictive QSAR Modeling Workflow, Model Applicability Domains, and Virtual Screening. Current Pharmaceutical Design, 2007, 13, 3494-3504.	1.9	369
13	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
14	Autoimmunity is triggered by cPR-3(105â€"201), a protein complementary to human autoantigen proteinase-3. Nature Medicine, 2004, 10, 72-79.	30.7	348
15	Quantitative Nanostructureâ^'Activity Relationship Modeling. ACS Nano, 2010, 4, 5703-5712.	14.6	342
16	Cross-Validated R2-Guided Region Selection for Comparative Molecular Field Analysis: A Simple Method To Achieve Consistent Results. Journal of Medicinal Chemistry, 1995, 38, 1060-1066.	6.4	296
17	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
18	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258

#	Article	IF	Citations
19	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling?. Journal of Chemical Information and Modeling, 2012, 52, 2570-2578.	5.4	232
20	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	5.4	228
21	A Novel Automated Lazy Learning QSAR (ALL-QSAR) Approach:â€‰ Method Development, Applications, and Virtual Screening of Chemical Databases Using Validated ALL-QSAR Models. Journal of Chemical Information and Modeling, 2006, 46, 1984-1995.	5.4	227
22	Quantitative Structureâ^'Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	3.3	210
23	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	6.7	209
24	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
25	Predictive QSAR modeling based on diversity sampling of experimental datasets for the training and test set selection. Molecular Diversity, 2000, 5, 231-243.	3.9	198
26	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	3.3	190
27	Phantom PAINS: Problems with the Utility of Alerts for <u>P</u>an-<u>A</u>ssay <u>IN</u>terference Compound<u>S</u>. Journal of Chemical Information and Modeling, 2017, 57, 417-427.	5.4	188
28	QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914.	3.5	163
29	A bibliometric review of drug repurposing. Drug Discovery Today, 2018, 23, 661-672.	6.4	163
30	Development and Validation ofk-Nearest-Neighbor QSPR Models of Metabolic Stability of Drug Candidates. Journal of Medicinal Chemistry, 2003, 46, 3013-3020.	6.4	162
31	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	2.5	159
32	Curation of chemogenomics data. Nature Chemical Biology, 2015, 11, 535-535.	8.0	158
33	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. Nature Communications, 2014, 5, 4757.	12.8	153
34	Delaunay Tessellation of Proteins: Four Body Nearest-Neighbor Propensities of Amino Acid Residues. Journal of Computational Biology, 1996, 3, 213-221.	1.6	152
35	Application of Predictive QSAR Models to Database Mining:â€‰ Identification and Experimental Validation of Novel Anticonvulsant Compounds. Journal of Medicinal Chemistry, 2004, 47, 2356-2364.	6.4	148
36	Three new consensus QSAR models for the prediction of Ames genotoxicity. Mutagenesis, 2004, 19, 365-377.	2.6	141

#	Article	IF	Citations
37	Quantitative Structureâ^'Activity Relationship Analysis of Functionalized Amino Acid Anticonvulsant Agents Using k Nearest Neighbor and Simulated Annealing PLS Methods. Journal of Medicinal Chemistry, 2002, 45, 2811-2823.	6.4	139
38	Combinatorial QSAR Modeling of P-Glycoprotein Substrates. Journal of Chemical Information and Modeling, 2006, 46, 1245-1254.	5.4	136
39	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	4.2	131
40	Systems chemical biology. Nature Chemical Biology, 2007, 3, 447-450.	8.0	129
41	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
42	QSAR Modeling of Human Serum Protein Binding with Several Modeling Techniques Utilizing Structureâ^'Information Representation. Journal of Medicinal Chemistry, 2006, 49, 7169-7181.	6.4	123
43	Novel Chirality Descriptors Derived from Molecular Topology. Journal of Chemical Information and Computer Sciences, 2001, 41, 147-158.	2.8	122
44	Four-body potentials reveal protein-specific correlations to stability changes caused by hydrophobic core mutations. Journal of Molecular Biology, 2001, 311, 625-638.	4.2	122
45	Cheminformatics Analysis of Assertions Mined from Literature That Describe Drug-Induced Liver Injury in Different Species. Chemical Research in Toxicology, 2010, 23, 171-183.	3.3	117
46	Integrative Chemicalâ€"Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	3.3	107
47	QSAR Modeling Using Chirality Descriptors Derived from Molecular Topology. Journal of Chemical Information and Computer Sciences, 2003, 43, 144-154.	2.8	105
48	Data Set Modelability by QSAR. Journal of Chemical Information and Modeling, 2014, 54, 1-4.	5.4	105
49	Modeling Liver-Related Adverse Effects of Drugs Using kNearest Neighbor Quantitative Structureâ^'Activity Relationship Method. Chemical Research in Toxicology, 2010, 23, 724-732.	3.3	104
50	Use of in Vitro HTS-Derived Concentrationâ€"Response Data as Biological Descriptors Improves the Accuracy of QSAR Models of in Vivo Toxicity. Environmental Health Perspectives, 2011, 119, 364-370.	6.0	103
51	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
52	Development of Quantitative Structureâ^'Binding Affinity Relationship Models Based on Novel Geometrical Chemical Descriptors of the Proteinâ^'Ligand Interfaces. Journal of Medicinal Chemistry, 2006, 49, 2713-2724.	6.4	99
53	Novel Inhibitors of Human Histone Deacetylase (HDAC) Identified by QSAR Modeling of Known Inhibitors, Virtual Screening, and Experimental Validation. Journal of Chemical Information and Modeling, 2009, 49, 461-476.	5.4	99
54	Quantitative Structureâ^'Activity Relationship Modeling of Dopamine D1 Antagonists Using Comparative Molecular Field Analysis, Genetic Algorithmsâ^'Partial Least-Squares, and K Nearest Neighbor Methods. Journal of Medicinal Chemistry, 1999, 42, 3217-3226.	6.4	98

#	Article	IF	Citations
55	Development of a four-body statistical pseudo-potential to discriminate native from non-native protein conformations. Bioinformatics, 2003, 19, 1540-1548.	4.1	98
56	Antitumor Agents. 199.â€Three-Dimensional Quantitative Structureâ^'Activity Relationship Study of the Colchicine Binding Site Ligands Using Comparative Molecular Field Analysis. Journal of Medicinal Chemistry, 2000, 43, 167-176.	6.4	97
57	Structure-Based Alignment and Comparative Molecular Field Analysis of Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 1996, 39, 5064-5071.	6.4	95
58	An updated review on drug-induced cholestasis: Mechanisms and investigation of physicochemical properties and pharmacokinetic parameters. Journal of Pharmaceutical Sciences, 2013, 102, 3037-3057.	3.3	95
59	Combinatorial QSAR of Ambergris Fragrance Compounds. Journal of Chemical Information and Computer Sciences, 2004, 44, 582-595.	2.8	93
60	Antitumor Agents. 163.â€Three-Dimensional Quantitative Structureâ^'Activity Relationship Study of 4â€˜-O-Demethylepipodophyllotoxin Analogs Using the Modified CoMFA/q2-GRS Approach. Journal of Medicinal Chemistry, 1996, 39, 1383-1395.	6.4	92
61	Rational Combinatorial Library Design. 2. Rational Design of Targeted Combinatorial Peptide Libraries Using Chemical Similarity Probe and the Inverse QSAR Approaches. Journal of Chemical Information and Computer Sciences, 1998, 38, 259-268.	2.8	90
62	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. Pharmaceutical Research, 2020, 37, 104.	3.5	90
63	Antitumor Agents. 213.â€Modeling of Epipodophyllotoxin Derivatives Using Variable SelectionkNearest Neighbor QSAR Method. Journal of Medicinal Chemistry, 2002, 45, 2294-2309.	6.4	89
64	Application of Validated QSAR Models of D1 Dopaminergic Antagonists for Database Mining. Journal of Medicinal Chemistry, 2005, 48, 7322-7332.	6.4	88
65	Rational Combinatorial Library Design. 1. Focus-2D:â€‰ A New Approach to the Design of Targeted Combinatorial Chemical Libraries. Journal of Chemical Information and Computer Sciences, 1998, 38, 251-258.	2.8	87
66	Antitumor Agents 252. Application of validated QSAR models to database mining: discovery of novel tylophorine derivatives as potential anticancer agents. Journal of Computer-Aided Molecular Design, 2007, 21, 97-112.	2.9	85
67	Use of Cell Viability Assay Data Improves the Prediction Accuracy of Conventional Quantitative Structureâ€"Activity Relationship Models of Animal Carcinogenicity. Environmental Health Perspectives, 2008, 116, 506-513.	6.0	82
68	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	2.1	82
69	Exploring Quantitative Nanostructure-Activity Relationships (QNAR) Modeling as a Tool for Predicting Biological Effects of Manufactured Nanoparticles. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 217-225.	1.1	79
70	Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 1013-1017.	5.4	79
71	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. Toxicology and Applied Pharmacology, 2013, 272, 67-76.	2.8	78
72	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	5.4	77

#	Article	IF	Citations
73	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	3.5	76
74	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for in silico nanosafety assessment. Computational and Structural Biotechnology Journal, 2020, 18, 583-602.	4.1	74
75	Quantitative structure - property relationship modeling of remote liposome loading of drugs. Journal of Controlled Release, 2012, 160, 147-157.	9.9	73
76	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	16.0	73
77	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. Toxicology and Applied Pharmacology, 2015, 284, 262-272.	2.8	72
78	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	3.0	72
79	Chembench: a cheminformatics workbench. Bioinformatics, 2010, 26, 3000-3001.	4.1	70
80	Comparing Graph Representations of Protein Structure for Mining Family-Specific Residue-Based Packing Motifs. Journal of Computational Biology, 2005, 12, 657-671.	1.6	67
81	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
82	Identification of the Descriptor Pharmacophores Using Variable Selection QSAR Applications to Database Mining. Current Pharmaceutical Design, 2001, 7, 599-612.	1.9	64
83	Predictive Modeling of Chemical Hazard by Integrating Numerical Descriptors of Chemical Structures and Short-term Toxicity Assay Data. Toxicological Sciences, 2012, 127, 1-9.	3.1	64
84	Novel ZE-Isomerism Descriptors Derived from Molecular Topology and Their Application to QSAR Analysis. Journal of Chemical Information and Computer Sciences, 2002, 42, 769-787.	2.8	63
85	QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays. Frontiers in Environmental Science, 2016, 4, .	3.3	63
86	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
87	Shedding the Light on Post-Vaccine Myocarditis and Pericarditis in COVID-19 and Non-COVID-19 Vaccine Recipients. Vaccines, 2021, 9, 1186.	4.4	61
88	Conformational Analysis of D1Dopamine Receptor Agonists:Â Pharmacophore Assessment and Receptor Mappingâ€. Journal of Medicinal Chemistry, 1996, 39, 285-296.	6.4	60
89	Rational Combinatorial Library Design. 3. Simulated Annealing Guided Evaluation (SAGE) of Molecular Diversity:â€‰ A Novel Computational Tool for Universal Library Design and Database Mining. Journal of Chemical Information and Computer Sciences, 1999, 39, 738-746.	2.8	59
90	A Novel Two-Step Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Work Flow for Predicting Acute Toxicity of Chemicals in Rodents. Environmental Health Perspectives, 2009, 117, 1257-1264.	6.0	59

#	Article	IF	Citations
91	Chemical toxicity prediction for major classes of industrial chemicals: Is it possible to develop universal models covering cosmetics, drugs, and pesticides?. Food and Chemical Toxicology, 2018, 112, 526-534.	3.6	57
92	QSAR Modeling of SARSâ€CoV M^{pro} Inhibitors Identifies Sufugolix, Cenicriviroc, Proglumetacin, and other Drugs as Candidates for Repurposing against SARSâ€CoVâ€2. Molecular Informatics, 2021, 40, e2000113.	2.5	57
93	kNearest Neighbors QSAR Modeling as a Variational Problem:Â Theory and Applications. Journal of Chemical Information and Modeling, 2005, 45, 777-785.	5.4	54
94	Chemometric Analysis of Ligand Receptor Complementarity:Â Identifying Complementary Ligands Based on Receptor Information (CoLiBRI). Journal of Chemical Information and Modeling, 2006, 46, 844-851.	5.4	54
95	Target, chemical and bioactivity databases â€“ integration is key. Drug Discovery Today: Technologies, 2006, 3, 357-365.	4.0	53
96	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. Toxicology and Applied Pharmacology, 2015, 284, 273-280.	2.8	53
97	New drug candidates for liposomal delivery identified by computer modeling of liposomes' remote loading and leakage. Journal of Controlled Release, 2017, 252, 18-27.	9.9	53
98	Conditional Toxicity Value (CTV) Predictor: An In Silico Approach for Generating Quantitative Risk Estimates for Chemicals. Environmental Health Perspectives, 2018, 126, 057008.	6.0	52
99	A motif found in propeptides and prohormones that may target them to secretory vesicles. Biochemical and Biophysical Research Communications, 1991, 174, 586-592.	2.1	51
100	Accurate prediction of the bound conformation of galanthamine in the active site of torpedo californica acetylcholinesterase using molecular docking. Journal of Molecular Graphics and Modelling, 2001, 19, 288-296.	2.4	51
101	Making sense from antisense: A review of experimental data and developing ideas on sense-antisense peptide recognition. Journal of Molecular Recognition, 1992, 5, 43-54.	2.1	49
102	Molecular Simulations of Î²-Sheet Twisting. Journal of Molecular Biology, 1996, 262, 283-293.	4.2	47
103	Quantitative High-Throughput Screening for Chemical Toxicity in a Population-Based In Vitro Model. Toxicological Sciences, 2012, 126, 578-588.	3.1	47
104	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	5.4	47
105	Application of free energy simulations to the binding of a transition-state-analogue inhibitor to HTV protease. Protein Engineering, Design and Selection, 1992, 5, 29-33.	2.1	45
106	Modelling the auxin-binding site of auxin-binding protein 1 of maize. Phytochemistry, 1994, 35, 1111-1123.	2.9	45
107	Relative Binding Free Energies of Peptide Inhibitors of HIV-1 Protease: The Influence of the Active Site Protonation State. Journal of Medicinal Chemistry, 1995, 38, 42-48.	6.4	44
108	Lattice protein folding with two and four-body statistical potentials. Proteins: Structure, Function and Bioinformatics, 2001, 43, 161-174.	2.6	44

#	Article	IF	Citations
109	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 7-13.	5.4	44
110	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	3.5	43
111	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structureâ€“Activity Relationship Models. Journal of Chemical Information and Modeling, 2018, 58, 1214-1223.	5.4	43
112	Chemocentric Informatics Approach to Drug Discovery: Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Ligands of 5-Hydroxytryptamine-6 Receptors and as Potential Cognition Enhancers. Journal of Medicinal Chemistry, 2012, 55, 5704-5719.	6.4	42
113	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	9.0	42
114	Scoring protein interaction decoys using exposed residues (SPIDER): A novel multibody interaction scoring function based on frequent geometric patterns of interfacial residues. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2207-2217.	2.6	41
115	Synthesis, Evaluation, and Comparative Molecular Field Analysis of 1-Phenyl-3-amino-1,2,3,4-tetrahydronaphthalenes as Ligands for Histamine H1 Receptors. Journal of Medicinal Chemistry, 1999, 42, 3041-3054.	6.4	40
116	Structure-based function inference using protein family-specific fingerprints. Protein Science, 2006, 15, 1537-1543.	7.6	39
117	Computer-aided design of liposomal drugs: In silico prediction and experimental validation of drug candidates for liposomal remote loading. Journal of Controlled Release, 2014, 173, 125-131.	9.9	39
118	PITPs as targets for selectively interfering with phosphoinositide signaling in cells. Nature Chemical Biology, 2014, 10, 76-84.	8.0	39
119	Antitumor Agents. 152. In vitro Inhibitory Activity of Etoposide Derivative NPF Against Human Tumor Cell Lines and a Study of Its Conformation by X-ray Crystallography, Molecular Modeling, and NMR Spectroscopy. Journal of Medicinal Chemistry, 1994, 37, 1460-1464.	6.4	38
120	Development, Validation, and Use of Quantitative Structureâ^'Activity Relationship Models of 5-Hydroxytryptamine (2B) Receptor Ligands to Identify Novel Receptor Binders and Putative Valvulopathic Compounds among Common Drugs. Journal of Medicinal Chemistry, 2010, 53, 7573-7586.	6.4	38
121	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	6.0	38
122	Antitumor Agents. 183. Syntheses, Conformational Analyses, and Antitubulin Activity of Allothiocolchicinoids. Journal of Organic Chemistry, 1998, 63, 4018-4025.	3.2	37
123	Differentiation of AmpC beta-lactamase binders vs. decoys using classification kNN QSAR modeling and application of the QSAR classifier to virtual screening. Journal of Computer-Aided Molecular Design, 2008, 22, 593-609.	2.9	37
124	Cheminformatics Meets Molecular Mechanics: A Combined Application of Knowledge-Based Pose Scoring and Physical Force Field-Based Hit Scoring Functions Improves the Accuracy of Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2012, 52, 16-28.	5.4	37
125	Reproducibility, sharing and progress in nanomaterial databases. Nature Nanotechnology, 2017, 12, 1111-1114.	31.5	37
126	Simplicial Neighborhood Analysis of Protein Packing (SNAPP): A Computational Geometry Approach to Studying Proteins. Methods in Enzymology, 2003, 374, 509-544.	1.0	36

#	Article	IF	Citations
127	Discovery of Geranylgeranyltransferase-I Inhibitors with Novel Scaffolds by the Means of Quantitative Structureâ"Activity Relationship Modeling, Virtual Screening, and Experimental Validation. Journal of Medicinal Chemistry, 2009, 52, 4210-4220.	6.4	36
128	Chemotext: A Publicly Available Web Server for Mining Drugâ€"Targetâ€"Disease Relationships in PubMed. Journal of Chemical Information and Modeling, 2018, 58, 212-218.	5.4	36
129	ROBOKOP KG and KGB: Integrated Knowledge Graphs from Federated Sources. Journal of Chemical Information and Modeling, 2019, 59, 4968-4973.	5.4	36
130	Quantitative structureâ"pharmacokinetic parameters relationships (QSPKR) analysis of antimicrobial agents in humans using simulated annealing kâ€nearestâ€neighbor and partial leastâ€square analysis methods**This paper was presented in part at the Annual Meeting of the American Association of Pharmaceutical Scientists in Toronto in 2003.. Journal of Pharmaceutical Sciences, 2004, 93, 2535-2544.	3.3	35
131	Combinatorial QSAR Modeling of Specificity and Subtype Selectivity of Ligands Binding to Serotonin Receptors 5HT1E and 5HT1F. Journal of Chemical Information and Modeling, 2008, 48, 997-1013.	5.4	35
132	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	6.7	35
133	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. Journal of Chemical Information and Modeling, 2021, 61, 653-663.	5.4	35
134	Prediction of binding affinity and efficacy of thyroid hormone receptor ligands using QSAR and structure-based modeling methods. Toxicology and Applied Pharmacology, 2014, 280, 177-189.	2.8	34
135	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. Science Advances, 2019, 5, eaav9784.	10.3	34
136	Novel ligands for the human histamine H1 receptor: Synthesis, pharmacology, and comparative molecular field analysis studies of 2-dimethylamino-5-(6)-phenyl-1,2,3,4-tetrahydronaphthalenes. Bioorganic and Medicinal Chemistry, 2006, 14, 6640-6658.	3.0	33
137	ROBOKOP: an abstraction layer and user interface for knowledge graphs to support question answering. Bioinformatics, 2019, 35, 5382-5384.	4.1	33
138	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	6.4	33
139	Free Energies for Folding and Refolding of Four Types of .beta. Turns: Simulation of the Role of D/L Chirality. Journal of the American Chemical Society, 1995, 117, 7592-7599.	13.7	32
140	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
141	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 3582-3594.	6.4	32
142	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	3.3	32
143	Discrete Molecular Dynamics Distinguishes Nativelike Binding Poses from Decoys in Difficult Targets. Biophysical Journal, 2012, 102, 144-151.	0.5	31
144	An Efficient Projection Protocol for Chemical Databases:â€‰ Singular Value Decomposition Combined with Truncated-Newton Minimization. Journal of Chemical Information and Computer Sciences, 2000, 40, 167-177.	2.8	30

#	Article	IF	Citations
145	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology, 2016, 10, 374-383.	3.0	29
146	Do crystal structures obviate the need for theoretical models of GPCRs for structureâ€based virtual screening?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1503-1521.	2.6	27
147	Computational Methods for Drug Discovery and Design. Journal of Medicinal Chemistry, 2016, 59, 1-1.	6.4	27
148	The ?random-coil? state of proteins: Comparison of database statistics and molecular simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 407-418.	2.6	26
149	Application of Quantitative Structureâ€“Activity Relationship Models of 5-HT_{1A} Receptor Binding to Virtual Screening Identifies Novel and Potent 5-HT_{1A} Ligands. Journal of Chemical Information and Modeling, 2014, 54, 634-647.	5.4	26
150	Learning from history: do not flatten the curve of antiviral research!. Drug Discovery Today, 2020, 25, 1604-1613.	6.4	26
151	Development of kNN QSAR Models for 3-Arylisoquinoline Antitumor Agents. Bulletin of the Korean Chemical Society, 2011, 32, 2397-2404.	1.9	26
152	Oy Vey! A Comment on â€œMachine Learning of Toxicological Big Data Enables Read-Across Structure Activity Relationships Outperforming Animal Test Reproducibilityâ€• Toxicological Sciences, 2019, 167, 3-4.	3.1	24
153	Diversity and Coverage of Structural Sublibraries Selected Using the SAGE and SCA Algorithms. Journal of Chemical Information and Computer Sciences, 2001, 41, 1470-1477.	2.8	23
154	Modeling of p38 mitogen-activated protein kinase inhibitors using the Catalystâ„¢ HypoGen and k-nearest neighbor QSAR methods. Journal of Molecular Graphics and Modelling, 2004, 23, 129-138.	2.4	23
155	Combined Application of Cheminformatics- and Physical Force Field-Based Scoring Functions Improves Binding Affinity Prediction for CSAR Data Sets. Journal of Chemical Information and Modeling, 2011, 51, 2027-2035.	5.4	23
156	Material informatics driven design and experimental validation of lead titanate as an aqueous solar photocathode. Materials Discovery, 2016, 6, 9-16.	3.3	23
157	Rational Principles of Compound Selection for Combinatorial Library Design. Combinatorial Chemistry and High Throughput Screening, 2002, 5, 111-23.	1.1	22
158	Why Academic Drug Discovery Makes Sense. Science, 2006, 313, 1235c-1236c.	12.6	22
159	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborativeâ„¢. Drug Discovery Today, 2014, 19, 1696-1698.	6.4	22
160	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	5.4	22
161	Using Graph Indices for the Analysis and Comparison of Chemical Datasets. Molecular Informatics, 2013, 32, 827-842.	2.5	21
162	Comparative Analysis of QSARâ€based vs. Chemical Similarity Based Predictors of GPCRs Binding Affinity. Molecular Informatics, 2016, 35, 36-41.	2.5	21

#	Article	IF	Citations
163	A novel approach for exposing and sharing clinical data: the Translator Integrated Clinical and Environmental Exposures Service. Journal of the American Medical Informatics Association: JAMIA, 2019, 26, 1064-1073.	4.4	21
164	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
165	Learning Drug-Disease-Target Embedding (DDTE) from knowledge graphs to inform drug repurposing hypotheses. Journal of Biomedical Informatics, 2021, 119, 103838.	4.3	21
166	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2013, 53, 1915-1922.	5.4	20
167	Curated Data In â€" Trustworthy In Silico Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing. ATLA Alternatives To Laboratory Animals, 2021, 49, 73-82.	1.0	20
168	DISTANCE-BASED IDENTIFICATION OF STRUCTURE MOTIFS IN PROTEINS USING CONSTRAINED FREQUENT SUBGRAPH MINING. , 2006, , .		18
169	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2012, , 1309-1342.		17
170	A systems chemical biology study of malate synthase and isocitrate lyase inhibition in Mycobacterium tuberculosis during active and NRP growth. Computational Biology and Chemistry, 2013, 47, 167-180.	2.3	17
171	An atypical heterotrimeric GÎ± protein has substantially reduced nucleotide binding but retains nucleotide-independent interactions with its cognate RGS protein and GÎ²Î³ dimer. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5204-5218.	3.5	17
172	Energetic decomposition of the Î±-helix-coil equilibrium of a dynamic model system. Biopolymers, 1998, 39, 479-489.	2.4	16
173	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	2.1	16
174	Synthesis and Structureâ€"Activity Relationships of DCLK1 Kinase Inhibitors Based on a 5,11-Dihydro-6H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6-one Scaffold. Journal of Medicinal Chemistry, 2020, 63, 7817-7826.	6.4	16
175	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. Annual Reports in Computational Chemistry, 2006, 2, 113-126.	1.7	15
176	Docking and Scoring with Target-Specific Pose Classifier Succeeds in Native-Like Pose Identification But Not Binding Affinity Prediction in the CSAR 2014 Benchmark Exercise. Journal of Chemical Information and Modeling, 2016, 56, 1032-1041.	5.4	15
177	COVID-KOP: integrating emerging COVID-19 data with the ROBOKOP database. Bioinformatics, 2021, 37, 586-587.	4.1	15
178	Knowledge-based approaches to drug discovery for rare diseases. Drug Discovery Today, 2022, 27, 490-502.	6.4	15
179	Short Communication: Cheminformatics Analysis to Identify Predictors of Antiviral Drug Penetration into the Female Genital Tract. AIDS Research and Human Retroviruses, 2014, 30, 1058-1064.	1.1	14
180	Target-Specific Native/Decoy Pose Classifier Improves the Accuracy of Ligand Ranking in the CSAR 2013 Benchmark. Journal of Chemical Information and Modeling, 2015, 55, 63-71.	5.4	14

#	Article	IF	Citations
181	A Systems Biology Workflow for Drug and Vaccine Repurposing: Identifying Small-Molecule BCG Mimics to Reduce or Prevent COVID-19 Mortality. Pharmaceutical Research, 2020, 37, 212.	3.5	14
182	Integrative Approaches for Predicting In Vivo Effects of Chemicals from their Structural Descriptors and the Results of Short-Term Biological Assays. Current Topics in Medicinal Chemistry, 2014, 14, 1356-1364.	2.1	14
183	Generating folded protein structures with a lattice chain growth algorithm. Journal of Chemical Physics, 2000, 113, 5511.	3.0	13
184	Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. Journal of the American Medical Informatics Association: JAMIA, 2016, 23, 968-978.	4.4	13
185	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2017, , 2303-2340.		13
186	Conserved coronavirus proteins as targets of broad-spectrum antivirals. Antiviral Research, 2022, 204, 105360.	4.1	13
187	Rational design of a threeâ€heptad coiledâ€coil protein and comparison by molecular dynamics simulation with the GCN4 coiled coil: Presence of interior threeâ€center hydrogen bonds. Protein Science, 1994, 3, 345-355.	7.6	12
188	Molecular simulation of alkyl boronic acids: Molecular mechanics and solvation free energy calculations. Journal of Computational Chemistry, 1994, 15, 333-345.	3.3	12
189	Distributed Chemical Computing Using ChemStar: An Open Source Java Remote Method Invocation Architecture Applied to Large Scale Molecular Data from PubChem. Journal of Chemical Information and Modeling, 2008, 48, 691-703.	5.4	12
190	Recent Trends in Statistical QSAR Modeling of Environmental Chemical Toxicity. Exs, 2012, 101, 381-411.	1.4	12
191	Visualization Environment for Federated Knowledge Graphs: Development of an Interactive Biomedical Query Language and Web Application Interface. JMIR Medical Informatics, 2020, 8, e17964.	2.6	12
192	Pseudotorsional OCCO backbone angle as a single descriptor of protein secondary structure. Protein Science, 1995, 4, 1633-1643.	7.6	11
193	A Turning Point For Bloodâ€"Brain Barrier Modeling. Pharmaceutical Research, 2009, 26, 1283-1284.	3.5	11
194	Local kernel canonical correlation analysis with application to virtual drug screening. Annals of Applied Statistics, 2011, 5, 2169-2196.	1.1	11
195	Identification of Tumor-Specific MRI Biomarkers Using Machine Learning (ML). Diagnostics, 2021, 11, 742.	2.6	11
196	Analyzing the Systems Biology Effects of COVID-19 mRNA Vaccines to Assess Their Safety and Putative Side Effects. Pathogens, 2022, 11, 743.	2.8	11
197	Evaluation of the relative stability of liganded versus ligand-free protein conformations using Simplicial Neighborhood Analysis of Protein Packing (SNAPP) method. Proteins: Structure, Function and Bioinformatics, 2004, 56, 828-838.	2.6	10
198	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. Biomolecules, 2020, 10, 913.	4.0	10

#	Article	IF	Citations
199	A Biomedical Knowledge Graph System to Propose Mechanistic Hypotheses for Real-World Environmental Health Observations: Cohort Study and Informatics Application. JMIR Medical Informatics, 2021, 9, e26714.	2.6	10
200	Identification of Sequence-Specific Tertiary Packing Motifs in Protein Structures using Delaunay Tessellation. Lecture Notes in Computational Science and Engineering, 2002, , 477-494.	0.3	10
201	Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing. Oncotarget, 2018, 9, 4758-4772.	1.8	10
202	HIVâ€1 protease function and structure studies with the simplicial neighborhood analysis of protein packing method. Proteins: Structure, Function and Bioinformatics, 2008, 73, 742-753.	2.6	9
203	Functional Neighbors: Inferring Relationships between Nonhomologous Protein Families Using Family-Specific Packing Motifs. IEEE Transactions on Information Technology in Biomedicine, 2010, 14, 1137-1143.	3.2	9
204	Cross-validated R2 guided region selection for CoMFA studies. Journal of Computer - Aided Molecular Design, 1998, 12/14, 57-69.	1.0	8
205	QSAR in drug discovery. , 2010, , 151-164.		8
206	Materials Informatics. Journal of Chemical Information and Modeling, 2018, 58, 2377-2379.	5.4	7
207	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2018, 58, 2203-2213.	5.4	7
208	Inter-Modular Linkers play a crucial role in governing the biosynthesis of non-ribosomal peptides. Bioinformatics, 2019, 35, 3584-3591.	4.1	7
209	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals. Artificial Intelligence in the Life Sciences, 2021, 1, 100028.	2.2	7
210	Generalized linear response method: Application to hydration free energy calculations. Journal of Computational Chemistry, 1999, 20, 749-759.	3.3	6
211	Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity. Molecular Informatics, 2015, 34, 160-170.	2.5	6
212	Joint Virtual Special Issue on Computational Toxicology. Journal of Chemical Information and Modeling, 2020, 60, 1069-1071.	5.4	6
213	QSAR/QSPR Revisited. , 0, , 465-495.		6
214	Calculation of the Relative Binding Affinity of Enzyme Inhibitors Using the Generalized Linear Response Method. Journal of Chemical Theory and Computation, 2006, 2, 1435-1443.	5.3	5
215	The Development of Novel Chemical Fragmentâ€Based Descriptors Using Frequent Common Subgraph Mining Approach and Their Application in QSAR Modeling. Molecular Informatics, 2014, 33, 201-215.	2.5	5
216	Modernization of Enoxaparin Molecular Weight Determination Using Homogeneous Standards. Pharmaceuticals, 2017, 10, 66.	3.8	5

#	Article	IF	Citations
217	Quantitative Structureâ€“Price Relationship (QS$R) Modeling and the Development of Economically Feasible Drug Discovery Projects. Journal of Chemical Information and Modeling, 2019, 59, 1306-1313.	5.4	5
218	ZINC Express: A Virtual Assistant for Purchasing Compounds Annotated in the ZINC Database. Journal of Chemical Information and Modeling, 2021, 61, 1033-1036.	5.4	5
219	COVID-19 Knowledge Extractor (COKE): A Curated Repository of Drugâ€“Target Associations Extracted from the CORD-19 Corpus of Scientific Publications on COVID-19. Journal of Chemical Information and Modeling, 2021, , .	5.4	5
220	Defining clinical outcome pathways. Drug Discovery Today, 2022, 27, 1671-1678.	6.4	5
221	Rational design of a targeted combinatorial chemical library with opiatelike activity. International Journal of Quantum Chemistry, 1998, 69, 65-75.	2.0	4
222	Materials Informatics. Journal of Chemical Information and Modeling, 2018, 58, 1313-1314.	5.4	4
223	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-48.		4
224	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	3.2	3
225	A semantic similarity based methodology for predicting protein-protein interactions: Evaluation with P53-interacting kinases. Journal of Biomedical Informatics, 2020, 111, 103579.	4.3	3
226	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. ACS Pharmacology and Translational Science, 2022, 5, 468-478.	4.9	3
227	Activity prediction and identification of misâ€annotated chemical compounds using extreme descriptors. Journal of Chemometrics, 2016, 30, 99-108.	1.3	2
228	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-38.		2
229	Explaining Drug-Discovery Hypotheses Using Knowledge-Graph Patterns. , 2021, , .		2
230	Semi-empirical calculations of intramolecular acyl transfer in cis-enols of O-aroyl acetylacetones. Computational and Theoretical Chemistry, 1995, 332, 85-91.	1.5	1
231	Functional Neighbors: Inferring Relationships between Non-Homologous Protein Families Using Family-Specific Packing Motifs. , 2008, , .		0
232	Drugging Protein-Protein Interfaces of a Supramolecular Assembly as a Means to Overcome Resistance to Active Site Thymidylate Synthase Inhibitors. Biophysical Journal, 2020, 118, 515a.	0.5	0
233	Moving Towards FAIR Data Practices in Pharmacy Education. American Journal of Pharmaceutical Education, 2021, , 8670.	2.1	0
234	Dataset Modelability by QSAR: Continuous Response Variable. , 2022, , 233-253.		0

#	Article	IF	Citations
235	Session Introduction. , 2004, , .		0
236	COMPUTER-AIDED COMBINATORIAL CHEMISTRY AND CHEMINFORMATICS. , 1999, , 553-4.		0
237	Biogeometry: applications of computational geometry to molecular structure. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2005, , 1-3.	0.7	0
238	Compact Walks: Taming Knowledge-Graph Embeddings with Domain- and Task-Specific Pathways. , 2022, , .		0