Alexander Tropsha

List of Publications by Year
in descending order

238 papers	25,164 citations	10351 72 h-index	7333 152 g-index
264 all docs	264 docs citations	264 times ranked	18136 citing authors

#	Article	IF	Citations
1	Beware of q2!. Journal of Molecular Graphics and Modelling, 2002, 20, 269-276.	1.3	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.	1.5	1,698
3	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
4	Best Practices for QSAR Model Development, Validation, and Exploitation. Molecular Informatics, 2010, 29, 476-488.	1.4	1,369
5	Deep reinforcement learning for de novo drug design. Science Advances, 2018, 4, eaap7885.	4.7	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.	2.5	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.	1.3	588
8	Chemical Basis of Interactions Between Engineered Nanoparticles and Biological Systems. Chemical Reviews, 2014, 114, 7740-7781.	23.0	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.	5.8	435
11	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
12	Predictive QSAR Modeling Workflow, Model Applicability Domains, and Virtual Screening. Current Pharmaceutical Design, 2007, 13, 3494-3504.	0.9	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.	2.5	350
14	Autoimmunity is triggered by cPR-3(105â€"201), a protein complementary to human autoantigen proteinase-3. Nature Medicine, 2004, 10, 72-79.	15.2	348
15	Quantitative Nanostructureâ^'Activity Relationship Modeling. ACS Nano, 2010, 4, 5703-5712.	7.3	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.	2.9	296
17	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
18	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	2.5	258

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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.	2.5	232
20	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	2.5	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.	2.5	227
22	Quantitative Structureâ^'Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	1.7	210
23	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	3.2	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.	2.5	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.	2.1	198
26	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	1.7	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.	2.5	188
28	QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914.	1.7	163
29	A bibliometric review of drug repurposing. Drug Discovery Today, 2018, 23, 661-672.	3.2	163
30	Development and Validation ofk-Nearest-Neighbor QSPR Models of Metabolic Stability of Drug Candidates. Journal of Medicinal Chemistry, 2003, 46, 3013-3020.	2.9	162
31	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	1.4	159
32	Curation of chemogenomics data. Nature Chemical Biology, 2015, 11, 535-535.	3.9	158
33	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. Nature Communications, 2014, 5, 4757.	5.8	153
34	Delaunay Tessellation of Proteins: Four Body Nearest-Neighbor Propensities of Amino Acid Residues. Journal of Computational Biology, 1996, 3, 213-221.	0.8	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.	2.9	148
36	Three new consensus QSAR models for the prediction of Ames genotoxicity. Mutagenesis, 2004, 19, 365-377.	1.0	141

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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.	2.9	139
38	Combinatorial QSAR Modeling of P-Glycoprotein Substrates. Journal of Chemical Information and Modeling, 2006, 46, 1245-1254.	2.5	136
39	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
40	Systems chemical biology. Nature Chemical Biology, 2007, 3, 447-450.	3.9	129
41	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	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.	2.9	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.	2.0	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.	1.7	117
46	Integrative Chemicalâ€"Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	1.7	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.	2.5	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.	1.7	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.	2.8	103
51	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	4.6	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.	2.9	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.	2.5	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.	2.9	98

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55	Development of a four-body statistical pseudo-potential to discriminate native from non-native protein conformations. Bioinformatics, 2003, 19, 1540-1548.	1.8	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.	2.9	97
57	Structure-Based Alignment and Comparative Molecular Field Analysis of Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 1996, 39, 5064-5071.	2.9	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.	1.6	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.	2.9	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.	1.7	90
63	Antitumor Agents. 213.â€Modeling of Epipodophyllotoxin Derivatives Using Variable SelectionkNearest Neighbor QSAR Method. Journal of Medicinal Chemistry, 2002, 45, 2294-2309.	2.9	89
64	Application of Validated QSAR Models of D1 Dopaminergic Antagonists for Database Mining. Journal of Medicinal Chemistry, 2005, 48, 7322-7332.	2.9	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.	1.3	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.	2.8	82
68	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	1.0	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.	0.6	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.	2.5	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.	1.3	78
72	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	2.5	77

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73	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	1.7	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.	1.9	74
75	Quantitative structure - property relationship modeling of remote liposome loading of drugs. Journal of Controlled Release, 2012, 160, 147-157.	4.8	73
76	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	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.	1.3	72
78	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	1.4	72
79	Chembench: a cheminformatics workbench. Bioinformatics, 2010, 26, 3000-3001.	1.8	70
80	Comparing Graph Representations of Protein Structure for Mining Family-Specific Residue-Based Packing Motifs. Journal of Computational Biology, 2005, 12, 657-671.	0.8	67
81	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	2.3	65
82	Identification of the Descriptor Pharmacophores Using Variable Selection QSAR Applications to Database Mining. Current Pharmaceutical Design, 2001, 7, 599-612.	0.9	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.	1.4	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, .	1.5	63
86	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
87	Shedding the Light on Post-Vaccine Myocarditis and Pericarditis in COVID-19 and Non-COVID-19 Vaccine Recipients. Vaccines, 2021, 9, 1186.	2.1	61
88	Conformational Analysis of D1Dopamine Receptor Agonists:Â Pharmacophore Assessment and Receptor Mappingâ€. Journal of Medicinal Chemistry, 1996, 39, 285-296.	2.9	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.	2.8	59

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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.	1.8	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.	1.4	57
93	kNearest Neighbors QSAR Modeling as a Variational Problem:Â Theory and Applications. Journal of Chemical Information and Modeling, 2005, 45, 777-785.	2.5	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.	2.5	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.	1.3	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.	4.8	53
98	Conditional Toxicity Value (CTV) Predictor: An In Silico Approach for Generating Quantitative Risk Estimates for Chemicals. Environmental Health Perspectives, 2018, 126, 057008.	2.8	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.	1.0	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.	1.3	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.	1.1	49
102	Molecular Simulations of Î²-Sheet Twisting. Journal of Molecular Biology, 1996, 262, 283-293.	2.0	47
103	Quantitative High-Throughput Screening for Chemical Toxicity in a Population-Based In Vitro Model. Toxicological Sciences, 2012, 126, 578-588.	1.4	47
104	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	2.5	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.	1.0	45
106	Modelling the auxin-binding site of auxin-binding protein 1 of maize. Phytochemistry, 1994, 35, 1111-1123.	1.4	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.	2.9	44
108	Lattice protein folding with two and four-body statistical potentials. Proteins: Structure, Function and Bioinformatics, 2001, 43, 161-174.	1.5	44

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109	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 7-13.	2.5	44
110	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	1.7	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.	2.5	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.	2.9	42
113	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	4.6	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.	1.5	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.	2.9	40
116	Structure-based function inference using protein family-specific fingerprints. Protein Science, 2006, 15, 1537-1543.	3.1	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.	4.8	39
118	PITPs as targets for selectively interfering with phosphoinositide signaling in cells. Nature Chemical Biology, 2014, 10, 76-84.	3.9	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.	2.9	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.	2.9	38
121	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	2.8	38
122	Antitumor Agents. 183. Syntheses, Conformational Analyses, and Antitubulin Activity of Allothiocolchicinoids. Journal of Organic Chemistry, 1998, 63, 4018-4025.	1.7	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.	1.3	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.	2.5	37
125	Reproducibility, sharing and progress in nanomaterial databases. Nature Nanotechnology, 2017, 12, 1111-1114.	15.6	37
126	Simplicial Neighborhood Analysis of Protein Packing (SNAPP): A Computational Geometry Approach to Studying Proteins. Methods in Enzymology, 2003, 374, 509-544.	0.4	36

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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.	2.9	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.	2.5	36
129	ROBOKOP KG and KGB: Integrated Knowledge Graphs from Federated Sources. Journal of Chemical Information and Modeling, 2019, 59, 4968-4973.	2.5	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.	1.6	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.	2.5	35
132	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	3.2	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.	2.5	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.	1.3	34
135	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. Science Advances, 2019, 5, eaav9784.	4.7	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.	1.4	33
137	ROBOKOP: an abstraction layer and user interface for knowledge graphs to support question answering. Bioinformatics, 2019, 35, 5382-5384.	1.8	33
138	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	3.2	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.	6.6	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.	1.4	32
141	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 3582-3594.	2.9	32
142	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	1.7	32
143	Discrete Molecular Dynamics Distinguishes Nativelike Binding Poses from Decoys in Difficult Targets. Biophysical Journal, 2012, 102, 144-151.	0.2	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

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145	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology, 2016, 10, 374-383.	1.6	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.	1.5	27
147	Computational Methods for Drug Discovery and Design. Journal of Medicinal Chemistry, 2016, 59, 1-1.	2.9	27
148	The ?random-coil? state of proteins: Comparison of database statistics and molecular simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 407-418.	1.5	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.	2.5	26
150	Learning from history: do not flatten the curve of antiviral research!. Drug Discovery Today, 2020, 25, 1604-1613.	3.2	26
151	Development of kNN QSAR Models for 3-Arylisoquinoline Antitumor Agents. Bulletin of the Korean Chemical Society, 2011, 32, 2397-2404.	1.0	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.	1.4	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.	1.3	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.	2.5	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.	0.6	22
158	Why Academic Drug Discovery Makes Sense. Science, 2006, 313, 1235c-1236c.	6.0	22
159	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborativeâ„¢. Drug Discovery Today, 2014, 19, 1696-1698.	3.2	22
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