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	Dataset Modelability by QSAR: Continuous Response Variable. , 2022, , 233-253.		0
2	Knowledge-based approaches to drug discovery for rare diseases. Drug Discovery Today, 2022, 27, 490-502.	3.2	15
3	Defining clinical outcome pathways. Drug Discovery Today, 2022, 27, 1671-1678.	3.2	5
4	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	2.8	38
5	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	73
6	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. ACS Pharmacology and Translational Science, 2022, 5, 468-478.	2.5	3
7	Compact Walks: Taming Knowledge-Graph Embeddings with Domain- and Task-Specific Pathways. , 2022, , .		0
8	Conserved coronavirus proteins as targets of broad-spectrum antivirals. Antiviral Research, 2022, 204, 105360.	1.9	13
9	Analyzing the Systems Biology Effects of COVID-19 mRNA Vaccines to Assess Their Safety and Putative Side Effects. Pathogens, 2022, 11, 743.	1.2	11
10	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
11	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	1.7	32
12	COVID-KOP: integrating emerging COVID-19 data with the ROBOKOP database. Bioinformatics, 2021, 37, 586-587.	1.8	15
13	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 7-13.	2.5	44
14	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
15	ZINC Express: A Virtual Assistant for Purchasing Compounds Annotated in the ZINC Database. Journal of Chemical Information and Modeling, 2021, 61, 1033-1036.	2.5	5
16	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
17	Identification of Tumor-Specific MRI Biomarkers Using Machine Learning (ML). Diagnostics, 2021, 11, 742.	1.3	11
18	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.	0.7	20

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19	Moving Towards FAIR Data Practices in Pharmacy Education. American Journal of Pharmaceutical Education, 2021, , 8670.	0.7	0
20	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.	1.3	10
21	Learning Drug-Disease-Target Embedding (DDTE) from knowledge graphs to inform drug repurposing hypotheses. Journal of Biomedical Informatics, 2021, 119, 103838.	2.5	21
22	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
23	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
24	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, , .	2.5	5
25	Explaining Drug-Discovery Hypotheses Using Knowledge-Graph Patterns. , 2021, , .		2
26	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.	1.6	7
27	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.	2.0	17
28	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.	1.7	14
29	Learning from history: do not flatten the curve of antiviral research!. Drug Discovery Today, 2020, 25, 1604-1613.	3.2	26
30	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	2.5	21
31	A semantic similarity based methodology for predicting protein-protein interactions: Evaluation with P53-interacting kinases. Journal of Biomedical Informatics, 2020, 111, 103579.	2.5	3
32	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. Pharmaceutical Research, 2020, 37, 104.	1.7	90
33	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.	2.9	16
34	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
35	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. Biomolecules, 2020, 10, 913.	1.8	10
36	Joint Virtual Special Issue on Computational Toxicology. Journal of Chemical Information and Modeling, 2020, 60, 1069-1071.	2.5	6

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37	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.	0.2	0
38	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
39	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	3.2	33
40	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	2.5	22
41	Visualization Environment for Federated Knowledge Graphs: Development of an Interactive Biomedical Query Language and Web Application Interface. JMIR Medical Informatics, 2020, 8, e17964.	1.3	12
42	ROBOKOP: an abstraction layer and user interface for knowledge graphs to support question answering. Bioinformatics, 2019, 35, 5382-5384.	1.8	33
43	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. Science Advances, 2019, 5, eaav9784.	4.7	34
44	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.	2.2	21
45	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.	2.5	5
46	Inter-Modular Linkers play a crucial role in governing the biosynthesis of non-ribosomal peptides. Bioinformatics, 2019, 35, 3584-3591.	1.8	7
47	ROBOKOP KG and KGB: Integrated Knowledge Graphs from Federated Sources. Journal of Chemical Information and Modeling, 2019, 59, 4968-4973.	2.5	36
48	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
49	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 3582-3594.	2.9	32
50	Materials Informatics. Journal of Chemical Information and Modeling, 2018, 58, 1313-1314.	2.5	4
51	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	3.2	35
52	A bibliometric review of drug repurposing. Drug Discovery Today, 2018, 23, 661-672.	3.2	163
53	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
54	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

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55	Materials Informatics. Journal of Chemical Information and Modeling, 2018, 58, 2377-2379.	2.5	7
56	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
57	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.	2.5	7
58	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
59	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	1.4	72
60	Deep reinforcement learning for de novo drug design. Science Advances, 2018, 4, eaap7885.	4.7	740
61	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	1.4	3
62	Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing. Oncotarget, 2018, 9, 4758-4772.	0.8	10
63	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	2.5	47
64	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
65	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
66	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2017, , 2303-2340.		13
67	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
68	Reproducibility, sharing and progress in nanomaterial databases. Nature Nanotechnology, 2017, 12, 1111-1114.	15.6	37
69	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
70	Universal fragment descriptors for predicting properties of inorganic crystals. Nature Communications, 2017, 8, 15679.	5.8	435
71	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	0.7	16
72	Modernization of Enoxaparin Molecular Weight Determination Using Homogeneous Standards. Pharmaceuticals, 2017, 10, 66.	1.7	5

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73	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
74	QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays. Frontiers in Environmental Science, 2016, 4, .	1.5	63
75	Material informatics driven design and experimental validation of lead titanate as an aqueous solar photocathode. Materials Discovery, 2016, 6, 9-16.	3.3	23
76	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.	2.5	15
77	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	4.6	42
78	Comparative Analysis of QSARâ€based vs. Chemical Similarity Based Predictors of GPCRs Binding Affinity. Molecular Informatics, 2016, 35, 36-41.	1.4	21
79	Activity prediction and identification of misâ€annotated chemical compounds using extreme descriptors. Journal of Chemometrics, 2016, 30, 99-108.	0.7	2
80	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	2.5	228
81	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	4.6	103
82	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	2.3	65
83	Computational Methods for Drug Discovery and Design. Journal of Medicinal Chemistry, 2016, 59, 1-1.	2.9	27
84	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology, 2016, 10, 374-383.	1.6	29
85	Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. Journal of the American Medical Informatics Association: JAMIA, 2016, 23, 968-978.	2.2	13
86	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-48.		4
87	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2016, , 1-38.		2
88	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	1.4	159
89	Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity. Molecular Informatics, 2015, 34, 160-170.	1.4	6
90	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

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91	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
92	Curation of chemogenomics data. Nature Chemical Biology, 2015, 11, 535-535.	3.9	158
93	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.	2.5	14
94	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	3.2	209
95	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. Nature Communications, 2014, 5, 4757.	5.8	153
96	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.	0.5	14
97	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
98	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
99	Data Set Modelability by QSAR. Journal of Chemical Information and Modeling, 2014, 54, 1-4.	2.5	105
100	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborativeâ„¢. Drug Discovery Today, 2014, 19, 1696-1698.	3.2	22
101	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.	1.4	5
102	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
103	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
104	Chemical Basis of Interactions Between Engineered Nanoparticles and Biological Systems. Chemical Reviews, 2014, 114, 7740-7781.	23.0	478
105	PITPs as targets for selectively interfering with phosphoinositide signaling in cells. Nature Chemical Biology, 2014, 10, 76-84.	3.9	39
106	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.	1.0	14
107	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	1.0	82
108	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2013, 53, 1915-1922.	2.5	20

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109	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
110	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
111	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	1.7	76
112	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.	1.1	17
113	Integrative Chemicalâ€"Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	1.7	107
114	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	2.5	77
115	The Use of Pseudo-Equilibrium Constant Affords Improved QSAR Models of Human Plasma Protein Binding. Pharmaceutical Research, 2013, 30, 1790-1798.	1.7	43
116	Using Graph Indices for the Analysis and Comparison of Chemical Datasets. Molecular Informatics, 2013, 32, 827-842.	1.4	21
117	Quantitative High-Throughput Screening for Chemical Toxicity in a Population-Based In Vitro Model. Toxicological Sciences, 2012, 126, 578-588.	1.4	47
118	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
119	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
120	Discrete Molecular Dynamics Distinguishes Nativelike Binding Poses from Decoys in Difficult Targets. Biophysical Journal, 2012, 102, 144-151.	0.2	31
121	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
122	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
123	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment. , 2012, , 1309-1342.		17
124	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
125	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
126	Quantitative structure - property relationship modeling of remote liposome loading of drugs. Journal of Controlled Release, 2012, 160, 147-157.	4.8	73

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127	Recent Trends in Statistical QSAR Modeling of Environmental Chemical Toxicity. Exs, 2012, 101, 381-411.	1.4	12
128	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	1.7	190
129	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
130	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
131	Local kernel canonical correlation analysis with application to virtual drug screening. Annals of Applied Statistics, 2011, 5, 2169-2196.	0.5	11
132	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
133	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
134	Development of kNN QSAR Models for 3-Arylisoquinoline Antitumor Agents. Bulletin of the Korean Chemical Society, 2011, 32, 2397-2404.	1.0	26
135	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
136	Functional Neighbors: Inferring Relationships between Nonhomologous Protein Families Using Family-Specific Packing Motifs. IEEE Transactions on Information Technology in Biomedicine, 2010, 14, 1137-1143.	3.6	9
137	Best Practices for QSAR Model Development, Validation, and Exploitation. Molecular Informatics, 2010, 29, 476-488.	1.4	1,369
138	QSAR in drug discovery. , 2010, , 151-164.		8
139	Chembench: a cheminformatics workbench. Bioinformatics, 2010, 26, 3000-3001.	1.8	70
140	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
141	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
142	Quantitative Nanostructureâ^'Activity Relationship Modeling. ACS Nano, 2010, 4, 5703-5712.	7.3	342
143	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
144	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

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145	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
146	A Turning Point For Bloodâ€“Brain Barrier Modeling. Pharmaceutical Research, 2009, 26, 1283-1284.	1.7	11
147	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
148	Quantitative Structureâ^'Activity Relationship Modeling of Rat Acute Toxicity by Oral Exposure. Chemical Research in Toxicology, 2009, 22, 1913-1921.	1.7	210
149	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
150	QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914.	1.7	163
151	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
152	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.	1.5	9
153	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
154	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	2.5	258
155	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
156	Functional Neighbors: Inferring Relationships between Non-Homologous Protein Families Using Family-Specific Packing Motifs. , 2008, , .		0
157	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.	2.5	12
158	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
159	Predictive QSAR Modeling Workflow, Model Applicability Domains, and Virtual Screening. Current Pharmaceutical Design, 2007, 13, 3494-3504.	0.9	369
160	Systems chemical biology. Nature Chemical Biology, 2007, 3, 447-450.	3.9	129
161	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
162	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. Annual Reports in Computational Chemistry, 2006, 2, 113-126.	0.9	15

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164	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
165	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
166	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
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