Alexander Tropsha

List of Publications by Year in Descending Order

235 papers	19,600 citations	66 h-index	136 g-index
264 ext. papers	22,267 ext. citations	7 avg, IF	7.16 L-index

#	Paper	IF	Citations
235	Dataset Modelability by QSAR: Continuous Response Variable **2022**, 233-253		
234	Allosteric binders of ACE2 are promising anti-SARS-CoV-2 agents. **2022**,		1
233	STopTox: An Alternative to Animal Testing for Acute Systemic and Topical Toxicity.. *Environmental Health Perspectives*, **2022**, 130, 27012	8.4	1
232	The transformational role of GPU computing and deep learning in drug discovery. *Nature Machine Intelligence*, **2022**, 4, 211-221	22.5	6
231	Shedding the Light on Post-Vaccine Myocarditis and Pericarditis in COVID-19 and Non-COVID-19 Vaccine Recipients. *Vaccines*, **2021**, 9,	5.3	17
230	ZINC Express: A Virtual Assistant for Purchasing Compounds Annotated in the ZINC Database. *Journal of Chemical Information and Modeling*, **2021**, 61, 1033-1036	6.1	1
229	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
228	Identification of Tumor-Specific MRI Biomarkers Using Machine Learning (ML). *Diagnostics*, **2021**, 11,	3.8	2
227	Curated Data In - Trustworthy 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	2.1	6
226	Moving Towards FAIR Data Practices in Pharmacy Education. *American Journal of Pharmaceutical Education*, **2021**, 8670	2.5	
225	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	3.6	1
224	QSAR Modeling of SARS-CoV M Inhibitors Identifies Sufugolix, Cenicriviroc, Proglumetacin, and other Drugs as Candidates for Repurposing against SARS-CoV-2. *Molecular Informatics*, **2021**, 40, e2000113	3.8	33
223	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. *Chemical Research in Toxicology*, **2021**, 34, 258-267	4	12
222	COVID-KOP: integrating emerging COVID-19 data with the ROBOKOP database. *Bioinformatics*, **2021**, 37, 586-587	7.2	6
221	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. *Journal of Chemical Information and Modeling*, **2021**, 61, 7-13	6.1	13
220	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	6.1	9
219	Learning Drug-Disease-Target Embedding (DDTE) from knowledge graphs to inform drug repurposing hypotheses. *Journal of Biomedical Informatics*, **2021**, 119, 103838	10.2	3

218	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
217	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		0
216	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. *Pharmaceutical Research*, **2020**, 37, 104	4.5	43
215	Synthesis and Structure-Activity Relationships of DCLK1 Kinase Inhibitors Based on a 5,11-Dihydro-6-benzo[]pyrimido[5,4-][1,4]diazepin-6-one Scaffold. *Journal of Medicinal Chemistry*, **2020**, 63, 7817-7826	8.3	9
214	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for nanosafety assessment. *Computational and Structural Biotechnology Journal*, **2020**, 18, 583-602	6.8	41
213	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. *Biomolecules*, **2020**, 10,	5.9	6
212	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
211	Visualization Environment for Federated Knowledge Graphs: Development of an Interactive Biomedical Query Language and Web Application Interface. *JMIR Medical Informatics*, **2020**, 8, e17964	3.6	4
210	Recent progress on cheminformatics approaches to epigenetic drug discovery. *Drug Discovery Today*, **2020**, 25, 2268-2276	8.8	14
209	An atypical heterotrimeric G protein has substantially reduced nucleotide binding but retains nucleotide-independent interactions with its cognate RGS protein and G dimer. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 5204-5218	3.6	7
208	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	4.5	6
207	Learning from history: do not flatten the curve of antiviral research!. *Drug Discovery Today*, **2020**, 25, 1604-1613	8.8	10
206	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. *Journal of Chemical Information and Modeling*, **2020**, 60, 4056-4063	6.1	10
205	A semantic similarity based methodology for predicting protein-protein interactions: Evaluation with P53-interacting kinases. *Journal of Biomedical Informatics*, **2020**, 111, 103579	10.2	
204	The Inorganic Crystal Structure Database (ICSD): A Tool for Materials Sciences **2019**, 41-54		2
203	From Topological Descriptors to Expert Systems: A Route to Predictable Materials **2019**, 107-147		2
202	Machine Learning Interatomic Potentials for Global Optimization and Molecular Dynamics Simulation **2019**, 253-288		2
201	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. *Science Advances*, **2019**, 5, eaav9784	14.3	21

200	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	8.6	12
199	Quantitative Structure-Price Relationship (QS$R) Modeling and the Development of Economically Feasible Drug Discovery Projects. *Journal of Chemical Information and Modeling*, **2019**, 59, 1306-1313	6.1	3
198	ROBOKOP: an abstraction layer and user interface for knowledge graphs to support question answering. *Bioinformatics*, **2019**, 35, 5382-5384	7.2	14
197	Modeling Materials Quantum Properties with Machine Learning **2019**, 171-179		1
196	Crystallography Open Database: History, Development, and Perspectives **2019**, 1-39		1
195	Pauling File: Toward a Holistic View **2019**, 55-106		5
194	Cognitive Chemistry: The Marriage of Machine Learning and Chemistry to Accelerate Materials Discovery **2019**, 223-251		
193	Automated Computation of Materials Properties **2019**, 181-222		1
192	A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE as Reference Database **2019**, 149-170		1
191	Inter-Modular Linkers play a crucial role in governing the biosynthesis of non-ribosomal peptides. *Bioinformatics*, **2019**, 35, 3584-3591	7.2	5
190	ROBOKOP KG and KGB: Integrated Knowledge Graphs from Federated Sources. *Journal of Chemical Information and Modeling*, **2019**, 59, 4968-4973	6.1	10
189	Oy Vey! A Comment on "Machine Learning of Toxicological Big Data Enables Read-Across Structure Activity Relationships Outperforming Animal Test Reproducibility". *Toxicological Sciences*, **2019**, 167, 3-4	4.4	11
188	Uncommon Data Sources for QSAR Modeling **2018**, 395-403		
187	Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors. *Journal of Medicinal Chemistry*, **2018**, 61, 3582-3594	8.3	21
186	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 2845-2859	8.3	20
185	Computational Tools for ADMET Profiling **2018**, 211-244		1
184	A bibliometric review of drug repurposing. *Drug Discovery Today*, **2018**, 23, 661-672	8.8	115
183	Chemotext: A Publicly Available Web Server for Mining Drug-Target-Disease Relationships in PubMed. *Journal of Chemical Information and Modeling*, **2018**, 58, 212-218	6.1	19

182	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	4.7	29
181	Deep reinforcement learning for de novo drug design. *Science Advances*, **2018**, 4, eaap7885	14.3	401
180	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. *Drug Safety*, **2018**, 41, 1059-1072	5.1	2
179	Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing. *Oncotarget*, **2018**, 9, 4758-4772	3.3	9
178	Conditional Toxicity Value (CTV) Predictor: An Approach for Generating Quantitative Risk Estimates for Chemicals. *Environmental Health Perspectives*, **2018**, 126, 057008	8.4	30
177	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structure-Activity Relationships. *Journal of Chemical Information and Modeling*, **2018**, 58, 2203-2213	6.1	4
176	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structure-Activity Relationship Models. *Journal of Chemical Information and Modeling*, **2018**, 58, 1214-1223	6.1	27
175	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science*, **2018**, 152, 134-145	3.2	51
174	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. *Journal of Chemical Information and Modeling*, **2017**, 57, 105-108	6.1	32
173	New drug candidates for liposomal delivery identified by computer modeling of liposomes' remote loading and leakage. *Journal of Controlled Release*, **2017**, 252, 18-27	11.7	37
172	Phantom PAINS: Problems with the Utility of Alerts for Pan-Assay INterference CompoundS. *Journal of Chemical Information and Modeling*, **2017**, 57, 417-427	6.1	152
171	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment **2017**, 2303-2340		9
170	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	6.1	49
169	Reproducibility, sharing and progress in nanomaterial databases. *Nature Nanotechnology*, **2017**, 12, 1111-1114	38.1	29
168	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	3.8	29
167	Universal fragment descriptors for predicting properties of inorganic crystals. *Nature Communications*, **2017**, 8, 15679	17.4	289
166	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. *American Journal of Pharmaceutical Education*, **2017**, 81, 46	2.5	12
165	Activity prediction and identification of mis-annotated chemical compounds using extreme descriptors. *Journal of Chemometrics*, **2016**, 30, 99-108	1.6	2

164	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. *Journal of Chemical Information and Modeling*, **2016**, 56, 1243-52	6.1	152
163	Alarms about structural alerts. *Green Chemistry*, **2016**, 18, 4348-4360	10	72
162	QSAR Modeling and Prediction of Drug-Drug Interactions. *Molecular Pharmaceutics*, **2016**, 13, 545-56	5.6	37
161	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. *Nanotoxicology*, **2016**, 10, 374-83	5.3	24
160	Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. *Journal of the American Medical Informatics Association: JAMIA*, **2016**, 23, 968-78	8.6	11
159	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment **2016**, 1-48		3
158	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment **2016**, 1-38		2
157	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
156	QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays. *Frontiers in Environmental Science*, **2016**, 4,	4.8	42
155	Material informatics driven design and experimental validation of lead titanate as an aqueous solar photocathode. *Materials Discovery*, **2016**, 6, 9-16		21
154	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, 1032-41	6.1	14
153	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. *Green Chemistry*, **2016**, 18, 6501-6515	10	28
152	Comparative Analysis of QSAR-based vs. Chemical Similarity Based Predictors of GPCRs Binding Affinity. *Molecular Informatics*, **2016**, 35, 36-41	3.8	15
151	Curation of chemogenomics data. *Nature Chemical Biology*, **2015**, 11, 535	11.7	118
150	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	6.1	14
149	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. *Chemistry of Materials*, **2015**, 27, 735-743	9.6	172
148	Pred-hERG: A Novel web-Accessible Computational Tool for Predicting Cardiac Toxicity. *Molecular Informatics*, **2015**, 34, 698-701	3.8	90
147	Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity. *Molecular Informatics*, **2015**, 34, 160-70	3.8	5

146	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, 273-80	4.6	41
145	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, 262-72	4.6	50
144	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, 125-31	11.7	29
143	QSAR modeling: where have you been? Where are you going to?. *Journal of Medicinal Chemistry*, **2014**, 57, 4977-5010	8.3	996
142	Data set modelability by QSAR. *Journal of Chemical Information and Modeling*, **2014**, 54, 1-4	6.1	72
141	Expanding the scope of drug repurposing in pediatrics: the Children's Pharmacy Collaborative. *Drug Discovery Today*, **2014**, 19, 1696-1698	8.8	17
140	The Development of Novel Chemical Fragment-Based Descriptors Using Frequent Common Subgraph Mining Approach and Their Application in QSAR Modeling. *Molecular Informatics*, **2014**, 33, 201-15	3.8	3
139	Prediction of binding affinity and efficacy of thyroid hormone receptor ligands using QSAR and structure-based modeling methods. *Toxicology and Applied Pharmacology*, **2014**, 280, 177-89	4.6	23
138	Application of quantitative structure-activity relationship models of 5-HT1A receptor binding to virtual screening identifies novel and potent 5-HT1A ligands. *Journal of Chemical Information and Modeling*, **2014**, 54, 634-47	6.1	18
137	Chemical basis of interactions between engineered nanoparticles and biological systems. *Chemical Reviews*, **2014**, 114, 7740-81	68.1	398
136	PITPs as targets for selectively interfering with phosphoinositide signaling in cells. *Nature Chemical Biology*, **2014**, 10, 76-84	11.7	27
135	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. *Nature Communications*, **2014**, 5, 4757	17.4	118
134	Short communication: cheminformatics analysis to identify predictors of antiviral drug penetration into the female genital tract. *AIDS Research and Human Retroviruses*, **2014**, 30, 1058-64	1.6	12
133	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, 1356-64	3	14
132	Tuning HERG out: antitarget QSAR models for drug development. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1399-415	3	63
131	Predicting binding affinity of CSAR ligands using both structure-based and ligand-based approaches. *Journal of Chemical Information and Modeling*, **2013**, 53, 1915-22	6.1	20
130	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	4.6	65
129	An updated review on drug-induced cholestasis: mechanisms and investigation of physicochemical properties and pharmacokinetic parameters. *Journal of Pharmaceutical Sciences*, **2013**, 102, 3037-57	3.9	80

128	Human intestinal transporter database: QSAR modeling and virtual profiling of drug uptake, efflux and interactions. *Pharmaceutical Research*, **2013**, 30, 996-1007	4.5	65
127	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, 167-80	3.6	14
126	Integrative chemical-biological read-across approach for chemical hazard classification. *Chemical Research in Toxicology*, **2013**, 26, 1199-208	4	83
125	Discovery of novel antimalarial compounds enabled by QSAR-based virtual screening. *Journal of Chemical Information and Modeling*, **2013**, 53, 475-92	6.1	61
124	The use of pseudo-equilibrium constant affords improved QSAR models of human plasma protein binding. *Pharmaceutical Research*, **2013**, 30, 1790-8	4.5	33
123	Using Graph Indices for the Analysis and Comparison of Chemical Datasets. *Molecular Informatics*, **2013**, 32, 827-42	3.8	15
122	Quantitative structure-property relationship modeling of remote liposome loading of drugs. *Journal of Controlled Release*, **2012**, 160, 147-57	11.7	62
121	Predictive modeling of chemical hazard by integrating numerical descriptors of chemical structures and short-term toxicity assay data. *Toxicological Sciences*, **2012**, 127, 1-9	4.4	57
120	Does rational selection of training and test sets improve the outcome of QSAR modeling?. *Journal of Chemical Information and Modeling*, **2012**, 52, 2570-8	6.1	169
119	Discrete molecular dynamics distinguishes nativelike binding poses from decoys in difficult targets. *Biophysical Journal*, **2012**, 102, 144-51	2.9	28
118	Do crystal structures obviate the need for theoretical models of GPCRs for structure-based virtual screening?. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1503-21	4.2	26
117	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, 2207-17	4.2	36
116	Predictive QSAR Modeling: Methods and Applications in Drug Discovery and Chemical Risk Assessment **2012**, 1309-1342		10
115	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, 5704-19	8.3	33
114	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	6.1	32
113	Quantitative high-throughput screening for chemical toxicity in a population-based in vitro model. *Toxicological Sciences*, **2012**, 126, 578-88	4.4	35
112	Recent trends in statistical QSAR modeling of environmental chemical toxicity. *Exs*, **2012**, 101, 381-411		8
111	Predicting drug-induced hepatotoxicity using QSAR and toxicogenomics approaches. *Chemical Research in Toxicology*, **2011**, 24, 1251-62	4	156

110	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, 2027-35	6.1	23
109	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
108	LOCAL KERNEL CANONICAL CORRELATION ANALYSIS WITH APPLICATION TO VIRTUAL DRUG SCREENING. *Annals of Applied Statistics*, **2011**, 5, 2169-2196	2.1	9
107	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, 217-25	1.3	71
106	Use of in vitro HTS-derived concentration-response data as biological descriptors improves the accuracy of QSAR models of in vivo toxicity. *Environmental Health Perspectives*, **2011**, 119, 364-70	8.4	88
105	Development of kNN QSAR Models for 3-Arylisoquinoline Antitumor Agents. *Bulletin of the Korean Chemical Society*, **2011**, 32, 2397-2404	1.2	24
104	Chembench: a cheminformatics workbench. *Bioinformatics*, **2010**, 26, 3000-1	7.2	65
103	Trust, but verify: on the importance of chemical structure curation in cheminformatics and QSAR modeling research. *Journal of Chemical Information and Modeling*, **2010**, 50, 1189-204	6.1	474
102	Development, validation, and use of quantitative structure-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, 7573-86	8.3	32
101	Quantitative nanostructure-activity relationship modeling. *ACS Nano*, **2010**, 4, 5703-12	16.7	291
100	Modeling liver-related adverse effects of drugs using knearest neighbor quantitative structure-activity relationship method. *Chemical Research in Toxicology*, **2010**, 23, 724-32	4	88
99	Recent Advances in Development, Validation, and Exploitation of QSAR Models **2010**, 505-534		6
98	Cheminformatics analysis of assertions mined from literature that describe drug-induced liver injury in different species. *Chemical Research in Toxicology*, **2010**, 23, 171-83	4	102
97	Applicability domains for classification problems: Benchmarking of distance to models for Ames mutagenicity set. *Journal of Chemical Information and Modeling*, **2010**, 50, 2094-111	6.1	169
96	Functional neighbors: inferring relationships between nonhomologous protein families using family-specific packing motifs. *IEEE Transactions on Information Technology in Biomedicine*, **2010**, 14, 1137-43		7
95	Best Practices for QSAR Model Development, Validation, and Exploitation. *Molecular Informatics*, **2010**, 29, 476-88	3.8	1041
94	A novel two-step hierarchical quantitative structure-activity relationship modeling work flow for predicting acute toxicity of chemicals in rodents. *Environmental Health Perspectives*, **2009**, 117, 1257-64	8.4	55
93	A turning point for blood-brain barrier modeling. *Pharmaceutical Research*, **2009**, 26, 1283-4	4.5	9

92	Discovery of geranylgeranyltransferase-I inhibitors with novel scaffolds by the means of quantitative structure-activity relationship modeling, virtual screening, and experimental validation. *Journal of Medicinal Chemistry*, **2009**, 52, 4210-20	8.3	32
91	Quantitative structure-activity relationship modeling of rat acute toxicity by oral exposure. *Chemical Research in Toxicology*, **2009**, 22, 1913-21	4	156
90	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, 461-76	6.1	85
89	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	6.1	31
88	Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. *Journal of Chemical Information and Modeling*, **2008**, 48, 766-84	6.1	222
87	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, 1733-46	6.1	296
86	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	6.1	10
85	Use of cell viability assay data improves the prediction accuracy of conventional quantitative structure-activity relationship models of animal carcinogenicity. *Environmental Health Perspectives*, **2008**, 116, 506-13	8.4	72
84	QSAR modeling of the blood-brain barrier permeability for diverse organic compounds. *Pharmaceutical Research*, **2008**, 25, 1902-14	4.5	137
83	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	4.2	32
82	HIV-1 protease function and structure studies with the simplicial neighborhood analysis of protein packing method. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 742-53	4.2	7
81	Predictive QSAR modeling workflow, model applicability domains, and virtual screening. *Current Pharmaceutical Design*, **2007**, 13, 3494-504	3.3	313
80	Systems chemical biology. *Nature Chemical Biology*, **2007**, 3, 447-50	11.7	116
79	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	4.2	76
78	Why academic drug discovery makes sense. *Science*, **2006**, 313, 1235-6	33.3	22
77	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. *Annual Reports in Computational Chemistry*, **2006**, 2, 113-126	1.8	14
76	Combinatorial QSAR modeling of P-glycoprotein substrates. *Journal of Chemical Information and Modeling*, **2006**, 46, 1245-54	6.1	124
75	QSAR modeling of human serum protein binding with several modeling techniques utilizing structure-information representation. *Journal of Medicinal Chemistry*, **2006**, 49, 7169-81	8.3	101

74	A novel automated lazy learning QSAR (ALL-QSAR) approach: method development, applications, and virtual screening of chemical databases using validated ALL-QSAR models. *Journal of Chemical Information and Modeling*, **2006**, 46, 1984-95	6.1	187
73	Development of quantitative structure-binding affinity relationship models based on novel geometrical chemical descriptors of the protein-ligand interfaces. *Journal of Medicinal Chemistry*, **2006**, 49, 2713-24	8.3	83
72	Target, chemical and bioactivity databases Integration is key. *Drug Discovery Today: Technologies*, **2006**, 3, 357-365	7.1	45
71	Calculation of the Relative Binding Affinity of Enzyme Inhibitors Using the Generalized Linear Response Method. *Journal of Chemical Theory and Computation*, **2006**, 2, 1435-43	6.4	5
70	Chemometric analysis of ligand receptor complementarity: identifying Complementary Ligands Based on Receptor Information (CoLiBRI). *Journal of Chemical Information and Modeling*, **2006**, 46, 844-51	6.1	44
69	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, 6640-58	3.4	27
68	Structure-based function inference using protein family-specific fingerprints. *Protein Science*, **2006**, 15, 1537-43	6.3	33
67	DISTANCE-BASED IDENTIFICATION OF STRUCTURE MOTIFS IN PROTEINS USING CONSTRAINED FREQUENT SUBGRAPH MINING **2006**,		11
66	Comparing graph representations of protein structure for mining family-specific residue-based packing motifs. *Journal of Computational Biology*, **2005**, 12, 657-71	1.7	57
65	kappa Nearest neighbors QSAR modeling as a variational problem: theory and applications. *Journal of Chemical Information and Modeling*, **2005**, 45, 777-85	6.1	44
64	Application of validated QSAR models of D1 dopaminergic antagonists for database mining. *Journal of Medicinal Chemistry*, **2005**, 48, 7322-32	8.3	80
63	Biogeometry: applications of computational geometry to molecular structure. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2005**, 1-3	1.3	
62	Autoimmunity is triggered by cPR-3(105-201), a protein complementary to human autoantigen proteinase-3. *Nature Medicine*, **2004**, 10, 72-9	50.5	283
61	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, 828-38	4.2	9
60	Quantitative structure-pharmacokinetic parameters relationships (QSPKR) analysis of antimicrobial agents in humans using simulated annealing k-nearest-neighbor and partial least-square analysis methods. *Journal of Pharmaceutical Sciences*, **2004**, 93, 2535-44	3.9	27
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