Alexander Tropsha

List of Publications by Citations

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	Beware of q2!. *Journal of Molecular Graphics and Modelling*, **2002**, 20, 269-76	2.8	2774
234	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		1447
233	Best Practices for QSAR Model Development, Validation, and Exploitation. *Molecular Informatics*, **2010**, 29, 476-88	3.8	1041
232	QSAR modeling: where have you been? Where are you going to?. *Journal of Medicinal Chemistry*, **2014**, 57, 4977-5010	8.3	996
231	Rational selection of training and test sets for the development of validated QSAR models. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 241-53	4.2	492
230	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
229	Deep reinforcement learning for de novo drug design. *Science Advances*, **2018**, 4, eaap7885	14.3	401
228	Chemical basis of interactions between engineered nanoparticles and biological systems. *Chemical Reviews*, **2014**, 114, 7740-81	68.1	398
227	Novel variable selection quantitative structure--property relationship approach based on the k-nearest-neighbor principle. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 185-94		378
226	Predictive QSAR modeling workflow, model applicability domains, and virtual screening. *Current Pharmaceutical Design*, **2007**, 13, 3494-504	3.3	313
225	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
224	Quantitative nanostructure-activity relationship modeling. *ACS Nano*, **2010**, 4, 5703-12	16.7	291
223	Universal fragment descriptors for predicting properties of inorganic crystals. *Nature Communications*, **2017**, 8, 15679	17.4	289
222	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
221	Cross-validated R2-guided region selection for comparative molecular field analysis: a simple method to achieve consistent results. *Journal of Medicinal Chemistry*, **1995**, 38, 1060-6	8.3	282
220	Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. *Journal of Chemical Information and Modeling*, **2008**, 48, 766-84	6.1	222
219	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206

218	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
217	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
216	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. *Chemistry of Materials*, **2015**, 27, 735-743	9.6	172
215	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
214	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
213	Predicting drug-induced hepatotoxicity using QSAR and toxicogenomics approaches. *Chemical Research in Toxicology*, **2011**, 24, 1251-62	4	156
212	Quantitative structure-activity relationship modeling of rat acute toxicity by oral exposure. *Chemical Research in Toxicology*, **2009**, 22, 1913-21	4	156
211	Predictive QSAR modeling based on diversity sampling of experimental datasets for the training and test set selection. *Molecular Diversity*, **2002**, 5, 231-43	3.1	155
210	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
209	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. *Journal of Chemical Information and Modeling*, **2016**, 56, 1243-52	6.1	152
208	QSAR modeling of the blood-brain barrier permeability for diverse organic compounds. *Pharmaceutical Research*, **2008**, 25, 1902-14	4.5	137
207	Delaunay tessellation of proteins: four body nearest-neighbor propensities of amino acid residues. *Journal of Computational Biology*, **1996**, 3, 213-21	1.7	136
206	Development and validation of k-nearest-neighbor QSPR models of metabolic stability of drug candidates. *Journal of Medicinal Chemistry*, **2003**, 46, 3013-20	8.3	134
205	Application of predictive QSAR models to database mining: identification and experimental validation of novel anticonvulsant compounds. *Journal of Medicinal Chemistry*, **2004**, 47, 2356-64	8.3	130
204	Three new consensus QSAR models for the prediction of Ames genotoxicity. *Mutagenesis*, **2004**, 19, 365-77	2.8	128
203	Combinatorial QSAR modeling of P-glycoprotein substrates. *Journal of Chemical Information and Modeling*, **2006**, 46, 1245-54	6.1	124
202	Curation of chemogenomics data. *Nature Chemical Biology*, **2015**, 11, 535	11.7	118
201	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. *Nature Communications*, **2014**, 5, 4757	17.4	118

200	Systems chemical biology. *Nature Chemical Biology*, **2007**, 3, 447-50	11.7	116
199	A bibliometric review of drug repurposing. *Drug Discovery Today*, **2018**, 23, 661-672	8.8	115
198	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
197	Quantitative structure-activity relationship analysis of functionalized amino acid anticonvulsant agents using k nearest neighbor and simulated annealing PLS methods. *Journal of Medicinal Chemistry*, **2002**, 45, 2811-23	8.3	113
196	Four-body potentials reveal protein-specific correlations to stability changes caused by hydrophobic core mutations. *Journal of Molecular Biology*, **2001**, 311, 625-38	6.5	106
195	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
194	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
193	Novel chirality descriptors derived from molecular topology. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 147-58		97
192	Antitumor agents. 199. Three-dimensional quantitative structure-activity relationship study of the colchicine binding site ligands using comparative molecular field analysis. *Journal of Medicinal Chemistry*, **2000**, 43, 167-76	8.3	91
191	Pred-hERG: A Novel web-Accessible Computational Tool for Predicting Cardiac Toxicity. *Molecular Informatics*, **2015**, 34, 698-701	3.8	90
190	QSAR modeling using chirality descriptors derived from molecular topology. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 144-54		89
189	Quantitative structure-activity relationship modeling of dopamine D(1) antagonists using comparative molecular field analysis, genetic algorithms-partial least-squares, and K nearest neighbor methods. *Journal of Medicinal Chemistry*, **1999**, 42, 3217-26	8.3	89
188	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
187	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
186	Structure-based alignment and comparative molecular field analysis of acetylcholinesterase inhibitors. *Journal of Medicinal Chemistry*, **1996**, 39, 5064-71	8.3	87
185	Development of a four-body statistical pseudo-potential to discriminate native from non-native protein conformations. *Bioinformatics*, **2003**, 19, 1540-8	7.2	86
184	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
183	Antitumor agents. 163. Three-dimensional quantitative structure-activity relationship study of 4'-O-demethylepipodophyllotoxin analogs using the modified CoMFA/q2-GRS approach. *Journal of Medicinal Chemistry*, **1996**, 39, 1383-95	8.3	85

182	Combinatorial QSAR of ambergris fragrance compounds. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 582-95		84
181	Integrative chemical-biological read-across approach for chemical hazard classification. *Chemical Research in Toxicology*, **2013**, 26, 1199-208	4	83
180	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
179	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, 259-68		81
178	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
177	Application of validated QSAR models of D1 dopaminergic antagonists for database mining. *Journal of Medicinal Chemistry*, **2005**, 48, 7322-32	8.3	80
176	Antitumor agents. 213. Modeling of epipodophyllotoxin derivatives using variable selection k nearest neighbor QSAR method. *Journal of Medicinal Chemistry*, **2002**, 45, 2294-309	8.3	79
175	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
174	Rational combinatorial library design. 1. Focus-2D: a new approach to the design of targeted combinatorial chemical libraries. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 251-8		75
173	Alarms about structural alerts. *Green Chemistry*, **2016**, 18, 4348-4360	10	72
172	Data set modelability by QSAR. *Journal of Chemical Information and Modeling*, **2014**, 54, 1-4	6.1	72
171	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
170	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
169	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
168	Human intestinal transporter database: QSAR modeling and virtual profiling of drug uptake, efflux and interactions. *Pharmaceutical Research*, **2013**, 30, 996-1007	4.5	65
167	Chembench: a cheminformatics workbench. *Bioinformatics*, **2010**, 26, 3000-1	7.2	65
166	Tuning HERG out: antitarget QSAR models for drug development. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1399-415	3	63
165	Quantitative structure-property relationship modeling of remote liposome loading of drugs. *Journal of Controlled Release*, **2012**, 160, 147-57	11.7	62

164	Discovery of novel antimalarial compounds enabled by QSAR-based virtual screening. *Journal of Chemical Information and Modeling*, **2013**, 53, 475-92	6.1	61
163	Identification of the descriptor pharmacophores using variable selection QSAR: applications to database mining. *Current Pharmaceutical Design*, **2001**, 7, 599-612	3.3	58
162	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
161	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
160	Conformational analysis of D1 dopamine receptor agonists: pharmacophore assessment and receptor mapping. *Journal of Medicinal Chemistry*, **1996**, 39, 285-96	8.3	57
159	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
158	Rational combinatorial library design. 3. Simulated annealing guided evaluation (SAGE) of molecular diversity: a novel computational tool for universal library design and database mining. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 738-46		52
157	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science*, **2018**, 152, 134-145	3.2	51
156	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
155	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
154	A motif found in propeptides and prohormones that may target them to secretory vesicles. *Biochemical and Biophysical Research Communications*, **1991**, 174, 586-92	3.4	47
153	Novel ZE-isomerism descriptors derived from molecular topology and their application to QSAR analysis. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 769-87		46
152	Target, chemical and bioactivity databases Integration is key. *Drug Discovery Today: Technologies*, **2006**, 3, 357-365	7.1	45
151	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, 288-96, 374-8	2.8	45
150	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
149	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
148	Molecular simulations of beta-sheet twisting. *Journal of Molecular Biology*, **1996**, 262, 283-93	6.5	44
147	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	2.6	44

146	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. *Pharmaceutical Research*, **2020**, 37, 104	4.5	43
145	Application of free energy simulations to the binding of a transition-state-analogue inhibitor to HIV protease. *Protein Engineering, Design and Selection*, **1992**, 5, 29-33	1.9	42
144	QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays. *Frontiers in Environmental Science*, **2016**, 4,	4.8	42
143	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
142	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
141	Lattice protein folding with two and four-body statistical potentials. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 161-74	4.2	41
140	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, 42-8	8.3	41
139	Modelling the auxin-binding site of auxin-binding protein 1 of maize. *Phytochemistry*, **1994**, 35, 1111-1123	4	40
138	Synthesis, evaluation, and comparative molecular field analysis of 1-phenyl-3-amino-1,2,3,4-tetrahydronaphthalenes as ligands for histamine H(1) receptors. *Journal of Medicinal Chemistry*, **1999**, 42, 3041-54	8.3	39
137	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
136	QSAR Modeling and Prediction of Drug-Drug Interactions. *Molecular Pharmaceutics*, **2016**, 13, 545-56	5.6	37
135	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
134	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
133	Quantitative high-throughput screening for chemical toxicity in a population-based in vitro model. *Toxicological Sciences*, **2012**, 126, 578-88	4.4	35
132	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, 1460-4	8.3	34
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130	The use of pseudo-equilibrium constant affords improved QSAR models of human plasma protein binding. *Pharmaceutical Research*, **2013**, 30, 1790-8	4.5	33
129	Structure-based function inference using protein family-specific fingerprints. *Protein Science*, **2006**, 15, 1537-43	6.3	33

128	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
127	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. *Journal of Chemical Information and Modeling*, **2017**, 57, 105-108	6.1	32
126	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
125	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
124	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
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	4.2	32
122	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
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120	Conditional Toxicity Value (CTV) Predictor: An Approach for Generating Quantitative Risk Estimates for Chemicals. *Environmental Health Perspectives*, **2018**, 126, 057008	8.4	30
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113	Antitumor Agents. 183. Syntheses, Conformational Analyses, and Antitubulin Activity of Allothiocolchicinoids. *Journal of Organic Chemistry*, **1998**, 63, 4018-4025	4.2	28
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110	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
109	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
108	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
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105	The □random-coil□state of proteins: Comparison of database statistics and molecular simulations. *Proteins: Structure, Function and Bioinformatics*, **1999**, 36, 407-418	4.2	25
104	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. *Nanotoxicology*, **2016**, 10, 374-83	5.3	24
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98	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. *Science Advances*, **2019**, 5, eaav9784	14.3	21
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94	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
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90	Expanding the scope of drug repurposing in pediatrics: the Children's Pharmacy Collaborative. *Drug Discovery Today*, **2014**, 19, 1696-1698	8.8	17
89	Shedding the Light on Post-Vaccine Myocarditis and Pericarditis in COVID-19 and Non-COVID-19 Vaccine Recipients. *Vaccines*, **2021**, 9,	5.3	17
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87	Energetic decomposition of the alpha-helix-coil equilibrium of a dynamic model system. *Biopolymers*, **1996**, 39, 479-89	2.2	15
86	Comparative Analysis of QSAR-based vs. Chemical Similarity Based Predictors of GPCRs Binding Affinity. *Molecular Informatics*, **2016**, 35, 36-41	3.8	15
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84	ROBOKOP: an abstraction layer and user interface for knowledge graphs to support question answering. *Bioinformatics*, **2019**, 35, 5382-5384	7.2	14
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82	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. *Annual Reports in Computational Chemistry*, **2006**, 2, 113-126	1.8	14
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80	Recent progress on cheminformatics approaches to epigenetic drug discovery. *Drug Discovery Today*, **2020**, 25, 2268-2276	8.8	14
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78	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
77	Rational principles of compound selection for combinatorial library design. *Combinatorial Chemistry and High Throughput Screening*, **2002**, 5, 111-23	1.3	13
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75	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. *Journal of Chemical Information and Modeling*, **2021**, 61, 7-13	6.1	13

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70	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. *Chemical Research in Toxicology*, **2021**, 34, 258-267	4	12
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