

Andreas Bender

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

281 papers	11,052 citations	55 h-index	96 g-index
318 ext. papers	12,960 ext. citations	5.7 avg, IF	6.46 L-index

#	Paper	IF	Citations
281	A community effort to assess and improve drug sensitivity prediction algorithms. <i>Nature Biotechnology</i> , 2014 , 32, 1202-12	44.5	447
280	Molecular similarity: a key technique in molecular informatics. <i>Organic and Biomolecular Chemistry</i> , 2004 , 2, 3204-18	3.9	446
279	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. <i>Journal of Computer-Aided Molecular Design</i> , 2011 , 25, 533-54	4.2	311
278	Recognizing pitfalls in virtual screening: a critical review. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 867-81	6.1	295
277	Integrating high-content screening and ligand-target prediction to identify mechanism of action. <i>Nature Chemical Biology</i> , 2008 , 4, 59-68	11.7	277
276	Similarity searching of chemical databases using atom environment descriptors (MOLPRINT 2D): evaluation of performance. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1708-18		265
275	Analysis of pharmacology data and the prediction of adverse drug reactions and off-target effects from chemical structure. <i>ChemMedChem</i> , 2007 , 2, 861-73	3.7	251
274	Diversity-oriented synthesis; a spectrum of approaches and results. <i>Organic and Biomolecular Chemistry</i> , 2008 , 6, 1149-58	3.9	248
273	How similar are similarity searching methods? A principal component analysis of molecular descriptor space. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 108-19	6.1	236
272	Multi-parameter phenotypic profiling: using cellular effects to characterize small-molecule compounds. <i>Nature Reviews Drug Discovery</i> , 2009 , 8, 567-78	64.1	227
271	Molecular similarity searching using atom environments, information-based feature selection, and a naïve Bayesian classifier. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 170-8		226
270	From in silico target prediction to multi-target drug design: current databases, methods and applications. <i>Journal of Proteomics</i> , 2011 , 74, 2554-74	3.9	214
269	Computational prediction of metabolism: sites, products, SAR, P450 enzyme dynamics, and mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 617-48	6.1	212
268	A community computational challenge to predict the activity of pairs of compounds. <i>Nature Biotechnology</i> , 2014 , 32, 1213-22	44.5	184
267	Bridging chemical and biological space: "target fishing" using 2D and 3D molecular descriptors. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 6802-10	8.3	158
266	Modeling promiscuity based on in vitro safety pharmacology profiling data. <i>ChemMedChem</i> , 2007 , 2, 874-80	3.7	156
265	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. <i>Bioinformatics</i> , 2018 , 34, 1538-1546	4.6	151

264	A discussion of measures of enrichment in virtual screening: comparing the information content of descriptors with increasing levels of sophistication. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 1369-75	6.1	145
263	Mapping adverse drug reactions in chemical space. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 3103-7	8.3	136
262	In silico target fishing: Predicting biological targets from chemical structure. <i>Drug Discovery Today: Technologies</i> , 2006 , 3, 413-421	7.1	135
261	Characterization of activity landscapes using 2D and 3D similarity methods: consensus activity cliffs. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 477-91	6.1	131
260	Gaining insight into off-target mediated effects of drug candidates with a comprehensive systems chemical biology analysis. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 308-17	6.1	130
259	Proteochemometric modeling as a tool to design selective compounds and for extrapolating to novel targets. <i>MedChemComm</i> , 2011 , 2, 16-30	5	124
258	In silico target predictions: defining a benchmarking data set and comparison of performance of the multiclass Naïve Bayes and Parzen-Rosenblatt window. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1957-66	6.1	115
257	Anti-MRSA agent discovery using diversity-oriented synthesis. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 2808-12	16.4	113
256	Development of a novel azaspirane that targets the Janus kinase-signal transducer and activator of transcription (STAT) pathway in hepatocellular carcinoma in vitro and in vivo. <i>Journal of Biological Chemistry</i> , 2014 , 289, 34296-307	5.4	111
255	Melting point prediction employing k-nearest neighbor algorithms and genetic parameter optimization. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 2412-22	6.1	111
254	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. <i>Drug Discovery Today</i> , 2016 , 21, 225-38	8.8	108
253	Properties and prediction of mitochondrial transit peptides from Plasmodium falciparum. <i>Molecular and Biochemical Parasitology</i> , 2003 , 132, 59-66	1.9	105
252	The discovery of antibacterial agents using diversity-oriented synthesis. <i>Chemical Communications</i> , 2009 , 2446-62	5.8	100
251	"Bayes affinity fingerprints" improve retrieval rates in virtual screening and define orthogonal bioactivity space: when are multitarget drugs a feasible concept?. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 2445-56	6.1	96
250	Diversity-oriented synthesis of macrocyclic peptidomimetics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 6793-8	11.5	95
249	General melting point prediction based on a diverse compound data set and artificial neural networks. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 581-90	6.1	92
248	Skeletal diversity construction via a branching synthetic strategy. <i>Chemical Communications</i> , 2006 , 3296-8	8.8	87
247	Chemogenomic data analysis: prediction of small-molecule targets and the advent of biological fingerprint. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2007 , 10, 719-31	1.3	84

246	Trisubstituted-Imidazoles Induce Apoptosis in Human Breast Cancer Cells by Targeting the Oncogenic PI3K/Akt/mTOR Signaling Pathway. <i>PLoS ONE</i> , 2016 , 11, e0153155	3.7	84
245	Relating GPCRs pharmacological space based on ligands chemical similarities. <i>Journal of Cheminformatics</i> , 2013 , 5,	8.6	78
244	In silico target prediction: identification of on- and off-targets for crop protection agents. <i>Journal of Cheminformatics</i> , 2013 , 5,	8.6	78
243	Ligand-target prediction using Winnow and naive Bayesian algorithms and the implications of overall performance statistics. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 2313-25	6.1	77
242	Target prediction utilising negative bioactivity data covering large chemical space. <i>Journal of Cheminformatics</i> , 2015 , 7, 51	8.6	76
241	Synthesis of 1,2-benzisoxazole tethered 1,2,3-triazoles that exhibit anticancer activity in acute myeloid leukemia cell lines by inhibiting histone deacetylases, and inducing p21 and tubulin acetylation. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 6157-65	3.4	74
240	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. <i>MedChemComm</i> , 2015 , 6, 24-50	5	74
239	Design, synthesis, and biological evaluation of an allosteric inhibitor of HSET that targets cancer cells with supernumerary centrosomes. <i>Chemistry and Biology</i> , 2013 , 20, 1399-410		74
238	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. <i>Journal of Cheminformatics</i> , 2015 , 7, 1	8.6	70
237	P-glycoprotein substrate models using support vector machines based on a comprehensive data set. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 1447-56	6.1	67
236	Scaffold Diversity Analysis of Compound Data Sets Using an Entropy-Based Measure. <i>QSAR and Combinatorial Science</i> , 2009 , 28, 1551-1560		67
235	The challenges involved in modeling toxicity data in silico: a review. <i>Current Pharmaceutical Design</i> , 2012 , 18, 1266-91	3.3	67
234	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. <i>Bioinformatics</i> , 2016 , 32, 85-95	7.2	60
233	Developments in toxicogenomics: understanding and predicting compound-induced toxicity from gene expression data. <i>Molecular Omics</i> , 2018 , 14, 218-236	4.4	60
232	Using transcriptomics to guide lead optimization in drug discovery projects: Lessons learned from the QSTAR project. <i>Drug Discovery Today</i> , 2015 , 20, 505-13	8.8	60
231	Plate-based diversity selection based on empirical HTS data to enhance the number of hits and their chemical diversity. <i>Journal of Biomolecular Screening</i> , 2009 , 14, 690-9		59
230	Benchmarking of protein descriptor sets in proteochemometric modeling (part 1): comparative study of 13 amino acid descriptor sets. <i>Journal of Cheminformatics</i> , 2013 , 5, 41	8.6	58
229	Prospective validation of a comprehensive in silico hERG model and its applications to commercial compound and drug databases. <i>ChemMedChem</i> , 2010 , 5, 716-29	3.7	57

228	Understanding false positives in reporter gene assays: in silico chemogenomics approaches to prioritize cell-based HTS data. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1319-27	6.1	57
227	Assessment of structural diversity in combinatorial synthesis. <i>Current Opinion in Chemical Biology</i> , 2005 , 9, 304-9	9.7	56
226	Novel synthetic biscoumarins target tumor necrosis factor- α in hepatocellular carcinoma in vitro and in vivo. <i>Journal of Biological Chemistry</i> , 2014 , 289, 31879-31890	5.4	54
225	How diverse are diversity assessment methods? A comparative analysis and benchmarking of molecular descriptor space. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 230-42	6.1	53
224	Novel synthetic coumarins that targets NF- κ B in Hepatocellular carcinoma. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 893-7	2.9	52
223	Circular fingerprints: flexible molecular descriptors with applications from physical chemistry to ADME. <i>IDrugs: the Investigational Drugs Journal</i> , 2006 , 9, 199-204		51
222	Understanding and classifying metabolite space and metabolite-likeness. <i>PLoS ONE</i> , 2011 , 6, e28966	3.7	49
221	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. <i>Journal of Cheminformatics</i> , 2013 , 5, 42	8.6	48
220	Chemogenomics approaches to rationalizing the mode-of-action of traditional Chinese and Ayurvedic medicines. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 661-73	6.1	46
219	Synthesis and characterization of novel 2-amino-chromene-nitriles that target Bcl-2 in acute myeloid leukemia cell lines. <i>PLoS ONE</i> , 2014 , 9, e107118	3.7	46
218	Molecular surface point environments for virtual screening and the elucidation of binding patterns (MOLPRINT 3D). <i>Journal of Medicinal Chemistry</i> , 2004 , 47, 6569-83	8.3	46
217	Which compound to select in lead optimization? Prospectively validated proteochemometric models guide preclinical development. <i>PLoS ONE</i> , 2011 , 6, e27518	3.7	44
216	Identifying novel adenosine receptor ligands by simultaneous proteochemometric modeling of rat and human bioactivity data. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 7010-20	8.3	42
215	Characterizing bitterness: identification of key structural features and development of a classification model. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 569-76	6.1	42
214	Modelling compound cytotoxicity using conformal prediction and PubChem HTS data. <i>Toxicology Research</i> , 2017 , 6, 73-80	2.6	40
213	A novel chemogenomics analysis of G protein-coupled receptors (GPCRs) and their ligands: a potential strategy for receptor de-orphanization. <i>BMC Bioinformatics</i> , 2010 , 11, 316	3.6	40
212	Deep Confidence: A Computationally Efficient Framework for Calculating Reliable Prediction Errors for Deep Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 1269-1281	6.1	40
211	Alpha shapes applied to molecular shape characterization exhibit novel properties compared to established shape descriptors. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2231-41	6.1	39

210	Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 1: Ways to make an impact, and why we are not there yet. <i>Drug Discovery Today</i> , 2021 , 26, 511-524	8.8	39
209	Applying synergy metrics to combination screening data: agreements, disagreements and pitfalls. <i>Drug Discovery Today</i> , 2019 , 24, 2286-2298	8.8	38
208	Identification of Novel Class of Triazolo-Thiadiazoles as Potent Inhibitors of Human Heparanase and their Anticancer Activity. <i>BMC Cancer</i> , 2017 , 17, 235	4.8	38
207	Significantly improved HIV inhibitor efficacy prediction employing proteochemometric models generated from antivirogram data. <i>PLoS Computational Biology</i> , 2013 , 9, e1002899	5	38
206	How similar are those molecules after all? Use two descriptors and you will have three different answers. <i>Expert Opinion on Drug Discovery</i> , 2010 , 5, 1141-51	6.2	37
205	"Virtual fragment linking": an approach to identify potent binders from low affinity fragment hits. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 2481-91	8.3	37
204	Screening of quinoline, 1,3-benzoxazine, and 1,3-oxazine-based small molecules against isolated methionyl-tRNA synthetase and A549 and HCT116 cancer cells including an in silico binding mode analysis. <i>Organic and Biomolecular Chemistry</i> , 2015 , 13, 9381-7	3.9	36
203	A-ring dihalogenation increases the cellular activity of combretastatin-templated tetrazoles. <i>ACS Medicinal Chemistry Letters</i> , 2012 , 3, 177-81	4.3	36
202	Flexible 3D pharmacophores as descriptors of dynamic biological space. <i>Journal of Molecular Graphics and Modelling</i> , 2007 , 26, 622-33	2.8	36
201	Handbook of Chemoinformatics Algorithms		35
200	A large descriptor set and a probabilistic kernel-based classifier significantly improve druglikeness classification. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1776-86	6.1	34
199	Novel Adamantanyl-Based Thiadiazolyl Pyrazoles Targeting EGFR in Triple-Negative Breast Cancer. <i>ACS Omega</i> , 2016 , 1, 1412-1424	3.9	34
198	Discovery of a small-molecule inhibitor of specific serine residue BAD phosphorylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E10505-E10514	11.5	34
197	Analysis of Iterative Screening with Stepwise Compound Selection Based on Novartis In-house HTS Data. <i>ACS Chemical Biology</i> , 2016 , 11, 1255-64	4.9	33
196	"Plate cherry picking": a novel semi-sequential screening paradigm for cheaper, faster, information-rich compound selection. <i>Journal of Biomolecular Screening</i> , 2007 , 12, 320-7		33
195	Development of Novel Triazolo-Thiadiazoles from Heterogeneous "Green" Catalysis as Protein Tyrosine Phosphatase 1B Inhibitors. <i>Scientific Reports</i> , 2015 , 5, 14195	4.9	32
194	Synthesis and characterization of novel oxazines and demonstration that they specifically target cyclooxygenase 2. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 2931-6	2.9	32
193	Proteochemometric modeling in a Bayesian framework. <i>Journal of Cheminformatics</i> , 2014 , 6, 35	8.6	32

192	A two-directional strategy for the diversity-oriented synthesis of macrocyclic scaffolds. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 7545-51	3.9	32
191	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. <i>Journal of Cheminformatics</i> , 2015 , 7, 45	8.6	31
190	Bayesian methods in virtual screening and chemical biology. <i>Methods in Molecular Biology</i> , 2011 , 672, 175-96	1.4	31
189	Support vector inductive logic programming outperforms the naive Bayes classifier and inductive logic programming for the classification of bioactive chemical compounds. <i>Journal of Computer-Aided Molecular Design</i> , 2007 , 21, 269-80	4.2	31
188	Improving Screening Efficiency through Iterative Screening Using Docking and Conformal Prediction. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 439-444	6.1	30
187	Toward Understanding the Cold, Hot, and Neutral Nature of Chinese Medicines Using in Silico Mode-of-Action Analysis. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 468-483	6.1	30
186	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. <i>Journal of Cheminformatics</i> , 2019 , 11, 41	8.6	29
185	Adamantyl-tethered-biphenylic compounds induce apoptosis in cancer cells by targeting Bcl homologs. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016 , 26, 1056-1060	2.9	29
184	Anti-MRSA Agent Discovery Using Diversity-Oriented Synthesis. <i>Angewandte Chemie</i> , 2008 , 120, 2850-2854	3.4	29
183	Chemoinformatics-based classification of prohibited substances employed for doping in sport. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 2369-80	6.1	29
182	A prospective cross-screening study on G-protein-coupled receptors: lessons learned in virtual compound library design. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 5311-25	8.3	28
181	Conformal Regression for Quantitative Structure-Activity Relationship Modeling-Quantifying Prediction Uncertainty. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1132-1140	6.1	27
180	Synergy Maps: exploring compound combinations using network-based visualization. <i>Journal of Cheminformatics</i> , 2015 , 7, 36	8.6	27
179	Metrabase: a cheminformatics and bioinformatics database for small molecule transporter data analysis and (Q)SAR modeling. <i>Journal of Cheminformatics</i> , 2015 , 7, 31	8.6	27
178	Microwave-assisted synthesis, characterization and cytotoxic studies of novel estrogen receptor β ligands towards human breast cancer cells. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 1804-1807	3.9	27
177	Proteochemometric modelling coupled to in silico target prediction: an integrated approach for the simultaneous prediction of polypharmacology and binding affinity/potency of small molecules. <i>Journal of Cheminformatics</i> , 2015 , 7, 15	8.6	26
176	Increased diversity of libraries from libraries: chemoinformatic analysis of bis-diazacyclic libraries. <i>Chemical Biology and Drug Design</i> , 2011 , 77, 328-42	2.9	26
175	Substructure mining of GPCR ligands reveals activity-class specific functional groups in an unbiased manner. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 348-60	6.1	26

174	Fishing the target of antitubercular compounds: in silico target deconvolution model development and validation. <i>Journal of Proteome Research</i> , 2009 , 8, 2788-98	5.6	26
173	Screening for dihydrofolate reductase inhibitors using MOLPRINT 2D, a fast fragment-based method employing the naïve Bayesian classifier: limitations of the descriptor and the importance of balanced chemistry in training and test sets. <i>Journal of Biomolecular Screening</i> , 2005 , 10, 658-66		26
172	Synthesis and in vitro evaluation of hydrazinyl phthalazines against malaria parasite, Plasmodium falciparum. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016 , 26, 3300-3306	2.9	25
171	Dynamic clustering threshold reduces conformer ensemble size while maintaining a biologically relevant ensemble. <i>Journal of Computer-Aided Molecular Design</i> , 2010 , 24, 675-86	4.2	25
170	Prediction of Antibiotic Interactions Using Descriptors Derived from Molecular Structure. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 3902-3912	8.3	24
169	eMolTox: prediction of molecular toxicity with confidence. <i>Bioinformatics</i> , 2018 , 34, 2508-2509	7.2	24
168	Synthesis, biological evaluation and in silico and in vitro mode-of-action analysis of novel dihydropyrimidones targeting PPAR- α <i>RSC Advances</i> , 2014 , 4, 45143-45146	3.7	24
167	A One Pot Synthesis of Novel Bioactive Tri-Substitute-Condensed-Imidazopyridines that Targets Snake Venom Phospholipase A2. <i>PLoS ONE</i> , 2015 , 10, e0131896	3.7	24
166	A multi-label approach to target prediction taking ligand promiscuity into account. <i>Journal of Cheminformatics</i> , 2015 , 7, 24	8.6	23
165	Improved Chemical Structure-Activity Modeling Through Data Augmentation. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2682-92	6.1	23
164	Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. <i>Integrative Biology (United Kingdom)</i> , 2014 , 6, 1023-33	3.7	23
163	Connecting gene expression data from connectivity map and in silico target predictions for small molecule mechanism-of-action analysis. <i>Molecular BioSystems</i> , 2015 , 11, 86-96		22
162	Understanding Cytotoxicity and Cytostaticity in a High-Throughput Screening Collection. <i>ACS Chemical Biology</i> , 2016 , 11, 3007-3023	4.9	22
161	Analyzing multitarget activity landscapes using protein-ligand interaction fingerprints: interaction cliffs. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 251-62	6.1	22
160	Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 2: a discussion of chemical and biological data. <i>Drug Discovery Today</i> , 2021 , 26, 1040-1052	8.8	22
159	Design, synthesis and evaluation of semi-synthetic triazole-containing caffeic acid analogues as 5-lipoxygenase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2015 , 101, 573-83	6.8	21
158	Synthesis of Structurally Diverse N-Substituted Quaternary-Carbon-Containing Small Molecules from α -Disubstituted Propargyl Amino Esters. <i>Chemistry - A European Journal</i> , 2018 , 24, 13681-13687	4.8	21
157	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 2000-2014	6.1	21

156	Comparing the Influence of Simulated Experimental Errors on 12 Machine Learning Algorithms in Bioactivity Modeling Using 12 Diverse Data Sets. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1413-25	6.1	21
155	Substructure-based virtual screening for adenosine A2A receptor ligands. <i>ChemMedChem</i> , 2011 , 6, 2302-317	3.1	21
154	A novel applicability domain technique for mapping predictive reliability across the chemical space of a QSAR: reliability-density neighbourhood. <i>Journal of Cheminformatics</i> , 2016 , 8,	8.6	21
153	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. <i>Molecular Informatics</i> , 2015 , 34, 357-66	3.8	20
152	Combining Aggregation with Pareto Optimization: A Case Study in Evolutionary Molecular Design. <i>Lecture Notes in Computer Science</i> , 2009 , 453-467	0.9	20
151	Use of ligand based models for protein domains to predict novel molecular targets and applications to triage affinity chromatography data. <i>Journal of Proteome Research</i> , 2009 , 8, 2575-85	5.6	19
150	How Consistent are Publicly Reported Cytotoxicity Data? Large-Scale Statistical Analysis of the Concordance of Public Independent Cytotoxicity Measurements. <i>ChemMedChem</i> , 2016 , 11, 57-71	3.7	19
149	Prediction of synergistic drug combinations. <i>Current Opinion in Systems Biology</i> , 2017 , 4, 24-28	3.2	18
148	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3330-3339	6.1	18
147	Orthologue chemical space and its influence on target prediction. <i>Bioinformatics</i> , 2018 , 34, 72-79	7.2	18
146	Multi-objective evolutionary design of adenosine receptor ligands. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 1713-21	6.1	18
145	Chemogenomics approaches for receptor deorphanization and extensions of the chemogenomics concept to phenotypic space. <i>Current Topics in Medicinal Chemistry</i> , 2011 , 11, 1964-77	3	18
144	Using Machine Learning to Predict Synergistic Antimalarial Compound Combinations With Novel Structures. <i>Frontiers in Pharmacology</i> , 2018 , 9, 1096	5.6	18
143	Which aspects of HTS are empirically correlated with downstream success?. <i>Current Opinion in Drug Discovery & Development</i> , 2008 , 11, 327-37		18
142	A Nano-MgO and Ionic Liquid-Catalyzed 'Green' Synthesis Protocol for the Development of Adamantyl-Imidazolo-Thiadiazoles as Anti-Tuberculosis Agents Targeting Sterol 14 β -Demethylase (CYP51). <i>PLoS ONE</i> , 2015 , 10, e0139798	3.7	17
141	Neighbours of cancer-related proteins have key influence on pathogenesis and could increase the drug target space for anticancer therapies. <i>Npj Systems Biology and Applications</i> , 2017 , 3, 2	5	16
140	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. <i>Future Medicinal Chemistry</i> , 2014 , 6, 2029-56	4.1	16
139	Diversity selection of compounds based on 'protein affinity fingerprints' improves sampling of bioactive chemical space. <i>Chemical Biology and Drug Design</i> , 2013 , 82, 252-66	2.9	16

138	Concordance analysis of microarray studies identifies representative gene expression changes in Parkinson's disease: a comparison of 33 human and animal studies. <i>BMC Neurology</i> , 2017 , 17, 58	3.1	15
137	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. <i>Briefings in Bioinformatics</i> , 2018 , 19, 277-285	13.4	15
136	Understanding the mode-of-action of Cassia auriculata via in silico and in vivo studies towards validating it as a long term therapy for type II diabetes. <i>Journal of Ethnopharmacology</i> , 2017 , 197, 61-72	5	15
135	Nano-cuprous oxide catalyzed one-pot synthesis of a carbazole-based STAT3 inhibitor: a facile approach via intramolecular C-N bond formation reactions. <i>RSC Advances</i> , 2016 , 6, 36775-36785	3.7	15
134	Identification of Novel Aurora Kinase A (AURKA) Inhibitors via Hierarchical Ligand-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 36-47	6.1	15
133	Novel benzoxazine-based aglycones block glucose uptake in vivo by inhibiting glycosidases. <i>PLoS ONE</i> , 2014 , 9, e102759	3.7	14
132	Efficient calculation of compound similarity based on maximum common subgraphs and its application to prediction of gene transcript levels. <i>International Journal of Bioinformatics Research and Applications</i> , 2013 , 9, 407-32	0.9	14
131	Mining protein dynamics from sets of crystal structures using "consensus structures". <i>Protein Science</i> , 2010 , 19, 742-52	6.3	14
130	Analysis of activity space by fragment fingerprints, 2D descriptors, and multitarget dependent transformation of 2D descriptors. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 1078-83	6.1	14
129	Fragment-Based Drug Discovery of Phosphodiesterase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 1415-1424	8.3	14
128	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. <i>Journal of Cheminformatics</i> , 2020 , 12, 39	8.6	13
127	Experimental confirmation of new drug-target interactions predicted by Drug Profile Matching. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 8377-88	8.3	13
126	Cheminformatics. <i>Communications of the ACM</i> , 2012 , 55, 65-75	2.5	13
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