Andreas Bender

List of Publications by Year
in descending order

320 papers	14,731 citations	19477 61 h-index	28046 106 g-index
375 all docs	375 docs citations	375 times ranked	16302 citing authors

#	Article	IF	Citations
1	Molecular similarity: a key technique in molecular informatics. Organic and Biomolecular Chemistry, 2004, 2, 3204.	2.9	538
2	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	3.1	479
3	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. Bioinformatics, 2018, 34, 1538-1546.	4.2	394
4	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	5.7	371
5	Integrating high-content screening and ligand-target prediction to identify mechanism of action. Nature Chemical Biology, 2008, 4, 59-68.	8.0	336
6	Similarity Searching of Chemical Databases Using Atom Environment Descriptors (MOLPRINT 2D):â€‰ Evaluation of Performance. Journal of Chemical Information and Computer Sciences, 2004, 44, 1708-1718.	2.8	310
7	Analysis of Pharmacology Data and the Prediction of Adverse Drug Reactions and Off-Target Effects from Chemical Structure. ChemMedChem, 2007, 2, 861-873.	3.4	294
8	How Similar Are Similarity Searching Methods? A Principal Component Analysis of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2009, 49, 108-119.	5.7	275
9	Diversity-oriented synthesis; a spectrum of approaches and results. Organic and Biomolecular Chemistry, 2008, 6, 1149.	2.9	272
10	Multi-parameter phenotypic profiling: using cellular effects to characterize small-molecule compounds. Nature Reviews Drug Discovery, 2009, 8, 567-578.	61.5	269
11	Computational Prediction of Metabolism: Sites, Products, SAR, P450 Enzyme Dynamics, and Mechanisms. Journal of Chemical Information and Modeling, 2012, 52, 617-648.	5.7	251
12	Molecular Similarity Searching Using Atom Environments, Information-Based Feature Selection, and a NaÃ¯ve Bayesian Classifier. Journal of Chemical Information and Computer Sciences, 2004, 44, 170-178.	2.8	250
13	From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574.	2.5	246
14	Bridging Chemical and Biological Space:Â â€œTarget Fishingâ€•Using 2D and 3D Molecular Descriptors. Journal of Medicinal Chemistry, 2006, 49, 6802-6810.	6.6	188
15	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. Drug Discovery Today, 2016, 21, 225-238.	6.6	174
16	Modeling Promiscuity Based on inâ€…vitro Safety Pharmacology Profiling Data. ChemMedChem, 2007, 2, 874-880.	3.4	173
17	A Discussion of Measures of Enrichment in Virtual Screening:â€‰ Comparing the Information Content of Descriptors with Increasing Levels of Sophistication. Journal of Chemical Information and Modeling, 2005, 45, 1369-1375.	5.7	172
18	Gaining Insight into Off-Target Mediated Effects of Drug Candidates with a Comprehensive Systems Chemical Biology Analysis. Journal of Chemical Information and Modeling, 2009, 49, 308-317.	5.7	161

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19	In silico target fishing: Predicting biological targets from chemical structure. Drug Discovery Today: Technologies, 2006, 3, 413-421.	4.2	160
20	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. Drug Discovery Today, 2021, 26, 511-524.	6.6	160
21	Melting Point Prediction Employing k-Nearest Neighbor Algorithms and Genetic Parameter Optimization. Journal of Chemical Information and Modeling, 2006, 46, 2412-2422.	5.7	158
22	Mapping Adverse Drug Reactions in Chemical Space. Journal of Medicinal Chemistry, 2009, 52, 3103-3107.	6.6	158
23	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. Journal of Biological Chemistry, 2014, 289, 34296-34307.	3.5	153
24	Low-carbohydrateâ€“high-protein diet and long-term survival in a general population cohort. European Journal of Clinical Nutrition, 2007, 61, 575-581.	2.9	152
25	Characterization of Activity Landscapes Using 2D and 3D Similarity Methods: Consensus Activity Cliffs. Journal of Chemical Information and Modeling, 2009, 49, 477-491.	5.7	147
26	Proteochemometric modeling as a tool to design selective compounds and for extrapolating to novel targets. MedChemComm, 2011, 2, 16-30.	3.4	143
27	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. Journal of Cheminformatics, 2015, 7, 1.	6.4	141
28	In Silico Target Predictions: Defining a Benchmarking Data Set and Comparison of Performance of the Multiclass NaÃ¯ve Bayes and Parzen-Rosenblatt Window. Journal of Chemical Information and Modeling, 2013, 53, 1957-1966.	5.7	132
29	Antiâ€MRSA Agent Discovery Using Diversityâ€Oriented Synthesis. Angewandte Chemie - International Edition, 2008, 47, 2808-2812.	14.8	126
30	â€œBayes Affinity Fingerprintsâ€•Improve Retrieval Rates in Virtual Screening and Define Orthogonal Bioactivity Space:â€‰ When Are Multitarget Drugs a Feasible Concept?. Journal of Chemical Information and Modeling, 2006, 46, 2445-2456.	5.7	125
31	Properties and prediction of mitochondrial transit peptides from Plasmodium falciparum. Molecular and Biochemical Parasitology, 2003, 132, 59-66.	1.1	120
32	Trisubstituted-Imidazoles Induce Apoptosis in Human Breast Cancer Cells by Targeting the Oncogenic PI3K/Akt/mTOR Signaling Pathway. PLoS ONE, 2016, 11, e0153155.	2.5	117
33	General Melting Point Prediction Based on a Diverse Compound Data Set and Artificial Neural Networks. Journal of Chemical Information and Modeling, 2005, 45, 581-590.	5.7	116
34	The discovery of antibacterial agents using diversity-oriented synthesis. Chemical Communications, 2009, , 2446.	4.2	113
35	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.4	112
36	Diversity-oriented synthesis of macrocyclic peptidomimetics. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6793-6798.	7.6	107

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37	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. Bioorganic and Medicinal Chemistry, 2015, 23, 6157-6165.	3.1	105
38	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.2	100
39	Design, Synthesis, and Biological Evaluation of an Allosteric Inhibitor of HSET that Targets Cancer Cells with Supernumerary Centrosomes. Chemistry and Biology, 2013, 20, 1399-1410.	6.2	99
40	Chemogenomic Data Analysis: Prediction of Small-Molecule Targets and the Advent of Biological Fingerprints. Combinatorial Chemistry and High Throughput Screening, 2007, 10, 719-731.	1.1	97
41	Identification of two sources of carbon monoxide in comet Haleâ€“Bopp. Nature, 1999, 399, 662-665.	36.2	96
42	Developments in toxicogenomics: understanding and predicting compound-induced toxicity from gene expression data. Molecular Omics, 2018, 14, 218-236.	2.8	94
43	Skeletal diversity construction via a branching synthetic strategy. Chemical Communications, 2006, , 3296.	4.2	93
44	Ligand-Target Prediction Using Winnow and Naive Bayesian Algorithms and the Implications of Overall Performance Statistics. Journal of Chemical Information and Modeling, 2008, 48, 2313-2325.	5.7	93
45	Prospective Validation of a Comprehensive In silico hERG Model and its Applications to Commercial Compound and Drug Databases. ChemMedChem, 2010, 5, 716-729.	3.4	91
46	Benchmarking of protein descriptor sets in proteochemometric modeling (part 1): comparative study of 13 amino acid descriptor sets. Journal of Cheminformatics, 2013, 5, 41.	6.4	90
47	Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 2: a discussion of chemical and biological data. Drug Discovery Today, 2021, 26, 1040-1052.	6.6	89
48	Scaffold Diversity Analysis of Compound Data Sets Using an Entropyâ€Based Measure. QSAR and Combinatorial Science, 2009, 28, 1551-1560.	1.5	86
49	Applying synergy metrics to combination screening data: agreements, disagreements and pitfalls. Drug Discovery Today, 2019, 24, 2286-2298.	6.6	84
50	Using transcriptomics to guide lead optimization in drug discovery projects: Lessons learned from the QSTAR project. Drug Discovery Today, 2015, 20, 505-513.	6.6	83
51	P-glycoprotein Substrate Models Using Support Vector Machines Based on a Comprehensive Data set. Journal of Chemical Information and Modeling, 2011, 51, 1447-1456.	5.7	82
52	Quantification of Collagen Organization in the Peripheral Human Cornea atÂMicron-Scale Resolution. Biophysical Journal, 2011, 101, 33-42.	0.5	81
53	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. Current Pharmaceutical Design, 2012, 18, 1266-1291.	1.9	80
54	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. Journal of Cheminformatics, 2013, 5, 42.	6.4	77

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55	Discovery of novel drug sensitivities in T-PLL by high-throughput ex vivo drug testing and mutation profiling. Leukemia, 2018, 32, 774-787.	7.5	77
56	Clinical predictors for the prognosis of myasthenia gravis. BMC Neurology, 2017, 17, 77.	1.8	70
57	Deep Confidence: A Computationally Efficient Framework for Calculating Reliable Prediction Errors for Deep Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 1269-1281.	5.7	70
58	How Diverse Are Diversity Assessment Methods? A Comparative Analysis and Benchmarking of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2014, 54, 230-242.	5.7	68
59	Plate-Based Diversity Selection Based on Empirical HTS Data to Enhance the Number of Hits and Their Chemical Diversity. SLAS Discovery, 2009, 14, 690-699.	2.8	67
60	Evaluation guidelines for machine learning tools in the chemical sciences. Nature Reviews Chemistry, 2022, 6, 428-442.	22.6	67
61	Understanding False Positives in Reporter Gene Assays:â€‰in Silico Chemogenomics Approaches To Prioritize Cell-Based HTS Data. Journal of Chemical Information and Modeling, 2007, 47, 1319-1327.	5.7	66
62	Novel Synthetic Biscoumarins Target Tumor Necrosis Factor-Î± in Hepatocellular Carcinoma in Vitro and in Vivo. Journal of Biological Chemistry, 2014, 289, 31879-31890.	3.5	65
63	Assessment of structural diversity in combinatorial synthesis. Current Opinion in Chemical Biology, 2005, 9, 304-309.	6.4	62
64	Designing Irreversible Inhibitorsâ€”Worth the Effort?. ChemMedChem, 2016, 11, 22-30.	3.4	61
65	Toward Understanding the Cold, Hot, and Neutral Nature of Chinese Medicines Using in Silico Mode-of-Action Analysis. Journal of Chemical Information and Modeling, 2017, 57, 468-483.	5.7	60
66	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. Journal of Cheminformatics, 2019, 11, 41.	6.4	60
67	Characterizing Bitterness:Â Identification of Key Structural Features and Development of a Classification Model. Journal of Chemical Information and Modeling, 2006, 46, 569-576.	5.7	59
68	Yeasts from Colombian Kumis as source of peptides with Angiotensin I converting enzyme (ACE) inhibitory activity in milk. International Journal of Food Microbiology, 2012, 159, 39-46.	4.8	59
69	Synthesis and Characterization of Novel 2-Amino-Chromene-Nitriles that Target Bcl-2 in Acute Myeloid Leukemia Cell Lines. PLoS ONE, 2014, 9, e107118.	2.5	55
70	Understanding and Classifying Metabolite Space and Metabolite-Likeness. PLoS ONE, 2011, 6, e28966.	2.5	54
71	Measuring customers benefits of click and collect. Journal of Services Marketing, 2018, 32, 430-442.	3.2	53
72	Metrabase: a cheminformatics and bioinformatics database for small molecule transporter data analysis and (Q)SAR modeling. Journal of Cheminformatics, 2015, 7, 31.	6.4	51

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73	Molecular Surface Point Environments for Virtual Screening and the Elucidation of Binding Patterns (MOLPRINT 3D). Journal of Medicinal Chemistry, 2004, 47, 6569-6583.	6.6	50
74	Algebraic properties of cryptosystem PGM. Journal of Cryptology, 1992, 5, 167-183.	2.9	49
75	Handbook of Chemoinformatics Algorithms. , 0, , .		49
76	Alpha Shapes Applied to Molecular Shape Characterization Exhibit Novel Properties Compared to Established Shape Descriptors. Journal of Chemical Information and Modeling, 2009, 49, 2231-2241.	5.7	48
77	Modelling compound cytotoxicity using conformal prediction and PubChem HTS data. Toxicology Research, 2017, 6, 73-80.	2.2	48
78	eMolTox: prediction of molecular toxicity with confidence. Bioinformatics, 2018, 34, 2508-2509.	4.2	48
79	Machine Learning Models for Human In Vivo Pharmacokinetic Parameters with In-House Validation. Molecular Pharmaceutics, 2021, 18, 4520-4530.	4.7	48
80	Flexible 3D pharmacophores as descriptors of dynamic biological space. Journal of Molecular Graphics and Modelling, 2007, 26, 622-633.	2.5	47
81	A novel chemogenomics analysis of G protein-coupled receptors (GPCRs) and their ligands: a potential strategy for receptor de-orphanization. BMC Bioinformatics, 2010, 11, 316.	2.7	47
82	Immunomodulation targeting of both Aî² and tau pathological conformers ameliorates Alzheimerâ€™s disease pathology in TgSwDI and 3xTg mouse models. Journal of Neuroinflammation, 2013, 10, 150.	7.4	47
83	Improving Screening Efficiency through Iterative Screening Using Docking and Conformal Prediction. Journal of Chemical Information and Modeling, 2017, 57, 439-444.	5.7	47
84	Prediction of Antibiotic Interactions Using Descriptors Derived from Molecular Structure. Journal of Medicinal Chemistry, 2017, 60, 3902-3912.	6.6	47
85	Which Compound to Select in Lead Optimization? Prospectively Validated Proteochemometric Models Guide Preclinical Development. PLoS ONE, 2011, 6, e27518.	2.5	47
86	How similar are those molecules after all? Use two descriptors and you will have three different answers. Expert Opinion on Drug Discovery, 2010, 5, 1141-1151.	5.1	46
87	Novel Adamantanyl-Based Thiadiazolyl Pyrazoles Targeting EGFR in Triple-Negative Breast Cancer. ACS Omega, 2016, 1, 1412-1424.	3.6	46
88	Discovery of a small-molecule inhibitor of specific serine residue BAD phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10505-E10514.	7.6	46
89	Integrating cell morphology with gene expression and chemical structure to aid mitochondrial toxicity detection. Communications Biology, 2022, 5, .	4.5	46
90	A-Ring Dihalogenation Increases the Cellular Activity of Combretastatin-Templated Tetrazoles. ACS Medicinal Chemistry Letters, 2012, 3, 177-181.	3.1	44

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91	Identification of Novel Class of Triazolo-Thiadiazoles as Potent Inhibitors of Human Heparanase and their Anticancer Activity. BMC Cancer, 2017, 17, 235.	2.6	44
92	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. Organic and Biomolecular Chemistry, 2015, 13, 9381-9387.	2.9	43
93	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	5.7	43
94	A Large Descriptor Set and a Probabilistic Kernel-Based Classifier Significantly Improve Druglikeness Classification. Journal of Chemical Information and Modeling, 2007, 47, 1776-1786.	5.7	42
95	Significantly Improved HIV Inhibitor Efficacy Prediction Employing Proteochemometric Models Generated From Antivirogram Data. PLoS Computational Biology, 2013, 9, e1002899.	3.1	42
96	Analysis of Iterative Screening with Stepwise Compound Selection Based on Novartis In-house HTS Data. ACS Chemical Biology, 2016, 11, 1255-1264.	3.6	42
97	Computational analyses of mechanism of action (MoA): data, methods and integration. RSC Chemical Biology, 2022, 3, 170-200.	4.2	42
98	Support vector inductive logic programming outperforms the naive Bayes classifier and inductive logic programming for the classification of bioactive chemical compounds. Journal of Computer-Aided Molecular Design, 2007, 21, 269-280.	3.1	41
99	Synthesis and characterization of novel oxazines and demonstration that they specifically target cyclooxygenase 2. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2931-2936.	2.3	40
100	Adamantyl-tethered-biphenylic compounds induce apoptosis in cancer cells by targeting Bcl homologs. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1056-1060.	2.3	40
101	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. Journal of Chemical Information and Modeling, 2019, 59, 3330-3339.	5.7	40
102	â€œVirtual Fragment Linkingâ€• An Approach To Identify Potent Binders from Low Affinity Fragment Hits. Journal of Medicinal Chemistry, 2008, 51, 2481-2491.	6.6	39
103	Unveiling a New Essential Cis Element for the Transactivation of theCYP3A4Gene by Xenobiotics. Molecular Pharmacology, 2009, 75, 677-684.	2.3	39
104	Improved Chemical Structureâ€“Activity Modeling Through Data Augmentation. Journal of Chemical Information and Modeling, 2015, 55, 2682-2692.	5.7	39
105	Microwave-assisted synthesis, characterization and cytotoxic studies of novel estrogen receptor Î± ligands towards human breast cancer cells. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1804-1807.	2.3	39
106	Comparison of structure- and ligand-based scoring functions for deep generative models: a GPCR case study. Journal of Cheminformatics, 2021, 13, 39.	6.4	39
107	Proteochemometric modeling in a Bayesian framework. Journal of Cheminformatics, 2014, 6, 35.	6.4	38
108	A novel applicability domain technique for mapping predictive reliability across the chemical space of a QSAR: reliability-density neighbourhood. Journal of Cheminformatics, 2016, 8, .	6.4	38

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109	Synthesis, biological evaluation and in silico and in vitro mode-of-action analysis of novel dihydropyrimidones targeting PPAR-Î³. RSC Advances, 2014, 4, 45143-45146.	3.7	37
110	DOCKSTRING: Easy Molecular Docking Yields Better Benchmarks for Ligand Design. Journal of Chemical Information and Modeling, 2022, 62, 3486-3502.	5.7	37
111	Dehydration-induced physical strains of cellulose microfibrils in plant cell walls. Carbohydrate Polymers, 2018, 197, 337-348.	10.5	36
112	Neonatal Catch Up Growth Increases Diabetes Susceptibility But Improves Behavioral and Cardiovascular Outcomes of Low Birth Weight Male Mice. Pediatric Research, 2009, 66, 53-58.	2.4	35
113	Comparison of Cellular Morphological Descriptors and Molecular Fingerprints for the Prediction of Cytotoxicity- and Proliferation-Related Assays. Chemical Research in Toxicology, 2021, 34, 422-437.	3.5	35
114	Peloruside A enhances apoptosis in H-ras-transformed cells and is cytotoxic to proliferating T cells. Apoptosis: an International Journal on Programmed Cell Death, 2004, 9, 785-796.	4.9	34
115	Flavobacterium compostarboris sp. nov., isolated from leaf-and-branch compost, and emended descriptions of Flavobacterium hercynium , Flavobacterium resistens and Flavobacterium johnsoniae. International Journal of Systematic and Evolutionary Microbiology, 2012, 62, 2018-2024.	1.8	34
116	â€œPlate Cherry Pickingâ€• A Novel Semi-Sequential Screening Paradigm for Cheaper, Faster, Information-Rich Compound Selection. Journal of Biomolecular Screening, 2007, 12, 320-327.	0.5	33
117	Substructure Mining of GPCR Ligands Reveals Activity-Class Specific Functional Groups in an Unbiased Manner. Journal of Chemical Information and Modeling, 2009, 49, 348-360.	5.7	33
118	Bayesian Methods in Virtual Screening and Chemical Biology. Methods in Molecular Biology, 2010, 672, 175-196.	0.0	33
119	Synergy Maps: exploring compound combinations using network-based visualization. Journal of Cheminformatics, 2015, 7, 36.	6.4	33
120	Antiâ€MRSA Agent Discovery Using Diversityâ€Oriented Synthesis. Angewandte Chemie, 2008, 120, 2850-2854.	2.1	32
121	A two-directional strategy for the diversity-oriented synthesis of macrocyclic scaffolds. Organic and Biomolecular Chemistry, 2012, 10, 7545.	2.9	32
122	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. Journal of Cheminformatics, 2015, 7, 45.	6.4	32
123	Prediction of In Vivo Pharmacokinetic Parameters and Timeâ€“Exposure Curves in Rats Using Machine Learning from the Chemical Structure. Molecular Pharmaceutics, 2022, 19, 1488-1504.	4.7	32
124	A multi-label approach to target prediction taking ligand promiscuity into account. Journal of Cheminformatics, 2015, 7, 24.	6.4	31
125	Design, synthesis and evaluation of semi-synthetic triazole-containing caffeic acid analogues as 5-lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2015, 101, 573-583.	5.7	31
126	Extracellular Sphingomyelinase Rv0888 of Mycobacterium tuberculosis Contributes to Pathological Lung Injury of Mycobacterium smegmatis in Mice via Inducing Formation of Neutrophil Extracellular Traps. Frontiers in Immunology, 2018, 9, 677.	4.9	31

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127	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. Journal of Cheminformatics, 2020, 12, 39.	6.4	31
128	Comparison of Chemical Structure and Cell Morphology Information for Multitask Bioactivity Predictions. Journal of Chemical Information and Modeling, 2021, 61, 1444-1456.	5.7	31
129	Screening for Dihydrofolate Reductase Inhibitors Using MOLPRINT 2D, a Fast Fragment-Based Method Employing the NaÃ¯ve Bayesian Classifier: Limitations of the Descriptor and the Importance of Balanced Chemistry in Training and Test Sets. Journal of Biomolecular Screening, 2005, 10, 658-666.	0.5	30
130	Chemoinformatics-Based Classification of Prohibited Substances Employed for Doping in Sport. Journal of Chemical Information and Modeling, 2006, 46, 2369-2380.	5.7	30
131	Increased Diversity of Libraries from Libraries: Chemoinformatic Analysis of Bisâ€Diazacyclic Libraries. Chemical Biology and Drug Design, 2011, 77, 328-342.	3.4	30
132	A Prospective Cross-Screening Study on G-Protein-Coupled Receptors: Lessons Learned in Virtual Compound Library Design. Journal of Medicinal Chemistry, 2012, 55, 5311-5325.	6.6	30
133	Proteochemometric modelling coupled to in silico target prediction: an integrated approach for the simultaneous prediction of polypharmacology and binding affinity/potency of small molecules. Journal of Cheminformatics, 2015, 7, 15.	6.4	30
134	Comparing the Influence of Simulated Experimental Errors on 12 Machine Learning Algorithms in Bioactivity Modeling Using 12 Diverse Data Sets. Journal of Chemical Information and Modeling, 2015, 55, 1413-1425.	5.7	29
135	Identification of HDAC6â€Selective Inhibitors of Low Cancer Cell Cytotoxicity. ChemMedChem, 2016, 11, 81-92.	3.4	29
136	A machine learning approach to the accurate prediction of monitor units for a compact proton machine. Medical Physics, 2018, 45, 2243-2251.	2.9	29
137	Dynamic clustering threshold reduces conformer ensemble size while maintaining a biologically relevant ensemble. Journal of Computer-Aided Molecular Design, 2010, 24, 675-686.	3.1	28
138	Connecting gene expression data from connectivity map and in silico target predictions for small molecule mechanism-of-action analysis. Molecular BioSystems, 2015, 11, 86-96.	2.8	28
139	Synthesis and in vitro evaluation of hydrazinyl phthalazines against malaria parasite, Plasmodium falciparum. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 3300-3306.	2.3	28
140	Prediction of synergistic drug combinations. Current Opinion in Systems Biology, 2017, 4, 24-28.	2.8	28
141	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. Journal of Chemical Information and Modeling, 2018, 58, 2000-2014.	5.7	28
142	Cell Morphological Profiling Enables High-Throughput Screening for PROteolysis TArgeting Chimera (PROTAC) Phenotypic Signature. ACS Chemical Biology, 2022, 17, 1733-1744.	3.6	28
143	Combining Aggregation with Pareto Optimization: A Case Study in Evolutionary Molecular Design. Lecture Notes in Computer Science, 2009, , 453-467.	1.0	27
144	Fishing the Target of Antitubercular Compounds: In Silico Target Deconvolution Model Development and Validation. Journal of Proteome Research, 2009, 8, 2788-2798.	3.8	27

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145	Multi-Objective Evolutionary Design of Adenosine Receptor Ligands. Journal of Chemical Information and Modeling, 2012, 52, 1713-1721.	5.7	27
146	Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. Integrative Biology (United Kingdom), 2014, 6, 1023-1033.	1.3	27
147	A One Pot Synthesis of Novel Bioactive Tri-Substitute-Condensed-Imidazopyridines that Targets Snake Venom Phospholipase A2. PLoS ONE, 2015, 10, e0131896.	2.5	27
148	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. Molecular Informatics, 2015, 34, 357-366.	2.7	27
149	Neighbours of cancer-related proteins have key influence on pathogenesis and could increase the drug target space for anticancer therapies. Npj Systems Biology and Applications, 2017, 3, 2.	3.0	25
150	Identification of Novel Aurora Kinase A (AURKA) Inhibitors via Hierarchical Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2018, 58, 36-47.	5.7	25
151	Substructureâ€Based Virtual Screening for Adenosine A_{2A} Receptor Ligands. ChemMedChem, 2011, 6, 2302-2311.	3.4	24
152	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. Journal of Ethnopharmacology, 2017, 197, 61-72.	4.2	24
153	Synthesis of Structurally Diverse Nâ€Substituted Quaternaryâ€Carbonâ€Containing Small Molecules from Î±,Î±â€Disubstituted Propargyl Amino Esters. Chemistry - A European Journal, 2018, 24, 13681-13687.	3.9	24
154	Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262.	5.7	23
155	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	6.5	22
156	Concordance analysis of microarray studies identifies representative gene expression changes in Parkinsonâ€™s disease: a comparison of 33 human and animal studies. BMC Neurology, 2017, 17, 58.	1.8	22
157	A Nano-MgO and Ionic Liquid-Catalyzed â€˜Greenâ€™ Synthesis Protocol for the Development of Adamantyl-Imidazolo-Thiadiazoles as Anti-Tuberculosis Agents Targeting Sterol 14Î±-Demethylase (CYP51). PLoS ONE, 2015, 10, e0139798.	2.5	21
158	Use of Ligand Based Models for Protein Domains To Predict Novel Molecular Targets and Applications To Triage Affinity Chromatography Data. Journal of Proteome Research, 2009, 8, 2575-2585.	3.8	20
159	A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria. Malaria Journal, 2018, 17, 160.	2.2	20
160	Experiments with Factor VIII Separated from Fibrinogen by Electrophoresis in Free Buffer Film. British Journal of Haematology, 1966, 12, 583-594.	2.7	19
161	Diversity Selection of Compounds Based on â€˜Protein Affinity Fingerprintsâ€™ Improves Sampling of Bioactive Chemical Space. Chemical Biology and Drug Design, 2013, 82, 252-266.	3.4	19
162	Extending In Silico Mechanism-of-Action Analysis by Annotating Targets with Pathways: Application to Cellular Cytotoxicity Readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	2.4	19

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163	Nano-cuprous oxide catalyzed one-pot synthesis of a carbazole-based STAT3 inhibitor: a facile approach via intramolecular Câ€“N bond formation reactions. RSC Advances, 2016, 6, 36775-36785.	3.7	19
164	Transcriptomics predicts compound synergy in drug and natural product treated glioblastoma cells. PLoS ONE, 2020, 15, e0239551.	2.5	19
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