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	From pixels to phenotypes: Integrating image-based profiling with cell health data as BioMorph features improves interpretability. Molecular Biology of the Cell, 2024, 35, .	2.5	3
2	Insights into Drug Cardiotoxicity from Biological and Chemical Data: The First Public Classifiers for FDA Drug-Induced Cardiotoxicity Rank. Journal of Chemical Information and Modeling, 2024, 64, 1172-1186.	5.7	7
3	Investigating strangeness enhancement with multiplicity in pp collisions using angular correlations. Journal of High Energy Physics, 2024, 2024, .	4.8	0
4	P393 Effect of filgotinib on anaemia in patients with Ulcerative Colitis in SELECTION. Journal of Crohn's and Colitis, 2023, 17, i525-i527.	1.3	1
5	Using Transcriptomics and Cell Morphology Data in Drug Discovery: The Long Road to Practice. ACS Medicinal Chemistry Letters, 2023, 14, 386-395.	3.1	6
6	Prediction of Compound Plasma Concentrationâ€“Time Profiles in Mice Using Random Forest. Molecular Pharmaceutics, 2023, 20, 3060-3072.	4.7	9
7	Explaining Bloodâ€“Brain Barrier Permeability of Small Molecules by Integrated Analysis of Different Transport Mechanisms. Journal of Medicinal Chemistry, 2023, 66, 7253-7267.	6.6	8
8	E-health security in big data of cloud computing in Jordanian healthcare sector. AIP Conference Proceedings, 2023, , .	1.0	0
9	Applications of Artificial Intelligence in Drug Design: Opportunities and Challenges. Methods in Molecular Biology, 2022, 2390, 1-59.	0.0	16
10	Computational analyses of mechanism of action (MoA): data, methods and integration. RSC Chemical Biology, 2022, 3, 170-200.	4.2	42
11	Deriving waveform parameters from calcium transients in human iPSC-derived cardiomyocytes to predict cardiac activity with machine learning. Stem Cell Reports, 2022, 17, 556-568.	4.7	8
12	Latent Variables Capture Pathway-Level Points of Departure in High-Throughput Toxicogenomic Data. Chemical Research in Toxicology, 2022, 35, 670-683.	3.5	5
13	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
14	Targeting Cell Death Mechanism Specifically in Triple Negative Breast Cancer Cell Lines. International Journal of Molecular Sciences, 2022, 23, 4784.	4.2	1
15	A systems genomics approach to uncover patient-specific pathogenic pathways and proteins in ulcerative colitis. Nature Communications, 2022, 13, 2299.	13.2	11
16	Evaluation guidelines for machine learning tools in the chemical sciences. Nature Reviews Chemistry, 2022, 6, 428-442.	22.6	67
17	DOCKSTRING: Easy Molecular Docking Yields Better Benchmarks for Ligand Design. Journal of Chemical Information and Modeling, 2022, 62, 3486-3502.	5.7	37
18	Cell Morphological Profiling Enables High-Throughput Screening for PROteolysis TArgeting Chimera (PROTAC) Phenotypic Signature. ACS Chemical Biology, 2022, 17, 1733-1744.	3.6	28

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19	Integrating cell morphology with gene expression and chemical structure to aid mitochondrial toxicity detection. Communications Biology, 2022, 5, .	4.5	46
20	Monomerization of Homodimeric Trefoil Factor 3 (TFF3) by an Aminonitrile Compound Inhibits TFF3-Dependent Cancer Cell Survival. ACS Pharmacology and Translational Science, 2022, 5, 761-773.	4.7	4
21	New Associations between Drug-Induced Adverse Events in Animal Models and Humans Reveal Novel Candidate Safety Targets. Chemical Research in Toxicology, 2021, 34, 438-451.	3.5	9
22	Systematic Analysis of Protein Targets Associated with Adverse Events of Drugs from Clinical Trials and Postmarketing Reports. Chemical Research in Toxicology, 2021, 34, 365-384.	3.5	15
23	Drug Combination Modeling. , 2021, , 269-282.		0
24	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
25	Combination of Ginsenosides Rb2 and Rg3 Promotes Angiogenic Phenotype of Human Endothelial Cells via PI3K/Akt and MAPK/ERK Pathways. Frontiers in Pharmacology, 2021, 12, 618773.	3.6	13
26	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
27	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
28	Nim: The Easy Winner!. , 2021, , 177-181.		0
29	Towards understanding antimicrobial activity, cytotoxicity and the mode of action of dichapetalins A and M using in silico and in vitro studies. Toxicon, 2021, 193, 28-37.	2.0	5
30	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
31	About time we banned live animal exports. Veterinary Record, 2021, 188, 274-274.	0.3	0
32	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
33	Transcriptional drug repositioning and cheminformatics approach for differentiation therapy of leukaemia cells. Scientific Reports, 2021, 11, 12537.	3.4	6
34	Disparities in Accessing and Reading Open Notes in the Emergency Department Upon Implementation of the 21st Century CURES Act. Annals of Emergency Medicine, 2021, 78, 593-598.	0.6	9
35	Computational Drug Repositioning for Ischemic Stroke: Neuroprotective Drug Discovery. Future Medicinal Chemistry, 2021, 13, 1271-1283.	2.4	4
36	Probabilistic Random Forest improves bioactivity predictions close to the classification threshold by taking into account experimental uncertainty. Journal of Cheminformatics, 2021, 13, 62.	6.4	12

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37	Prediction and identification of synergistic compound combinations against pancreatic cancer cells. IScience, 2021, 24, 103080.	4.1	2
38	In silico approaches in organ toxicity hazard assessment: Current status and future needs for predicting heart, kidney and lung toxicities. Computational Toxicology, 2021, 20, 100188.	3.4	13
39	In silico approaches in organ toxicity hazard assessment: Current status and future needs in predicting liver toxicity. Computational Toxicology, 2021, 20, 100187.	3.4	16
40	Machine Learning Models for Human In Vivo Pharmacokinetic Parameters with In-House Validation. Molecular Pharmaceutics, 2021, 18, 4520-4530.	4.7	48
41	Understanding Conditional Associations between ToxCast in Vitro Readouts and the Hepatotoxicity of Compounds Using Rule-Based Methods. Chemical Research in Toxicology, 2020, 33, 137-153.	3.5	6
42	Pathogenicity of Shiga Toxin Type 2e Escherichia coli in Pig Colibacillosis. Frontiers in Veterinary Science, 2020, 7, 545818.	2.3	14
43	Identification of Intrinsic Drug Resistance and Its Biomarkers in High-Throughput Pharmacogenomic and CRISPR Screens. Patterns, 2020, 1, 100065.	5.2	6
44	Comparison of Scaling Methods to Obtain Calibrated Probabilities of Activity for Proteinâ€“Ligand Predictions. Journal of Chemical Information and Modeling, 2020, 60, 4546-4559.	5.7	14
45	Transcriptomics predicts compound synergy in drug and natural product treated glioblastoma cells. PLoS ONE, 2020, 15, e0239551.	2.5	19
46	Establishing GPCR Targets of hMAO Active Anthraquinones from Cassia obtusifolia Linn Seeds Using In Silico and In Vitro Methods. ACS Omega, 2020, 5, 7705-7715.	3.6	5
47	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
48	QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction. Journal of Cheminformatics, 2020, 12, 41.	6.4	18
49	Fragmentâ€Based Ligand Discovery. , 2020, , 79-98.		2
50	EMDIP: An Entropy Measure to Discover Important Proteins in PPI networks. Computers in Biology and Medicine, 2020, 120, 103740.	7.3	6
51	Predicting and understanding synergistic pairwise compound combinations of Shexian Baoxin Pill (SBP) using network biology. Synergy, 2020, 11, 100073.	1.1	1
52	Wearing Time of Ankle-Foot Orthoses with Modular Shank Supply in Cerebral Palsy: A Descriptive Analysis in a Clinically Prospective Approach. Rehabilitation Research and Practice, 2019, 2019, 1-9.	0.7	6
53	Analyzing the costs (and benefits) of DNS, DoT, and DoH for the modern web. , 2019, , .		11
54	Triazoleâ€Pyridine Dicarbonitrile Targets Phosphodiesterase 4 to Induce Cytotoxicity in Lung Carcinoma Cells. Chemistry and Biodiversity, 2019, 16, e1900234.	2.2	7

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55	Applying synergy metrics to combination screening data: agreements, disagreements and pitfalls. Drug Discovery Today, 2019, 24, 2286-2298.	6.6	84
56	Sulfated Ceria Catalyzed Synthesis of Imidazopyridines and Their Implementation as DNA Minor Groove Binders. Chemistry and Biodiversity, 2019, 16, e1800435.	2.2	3
57	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
58	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. Journal of Chemical Information and Modeling, 2019, 59, 3330-3339.	5.7	40
59	Leveraging heterogeneous data from GHS toxicity annotations, molecular and protein target descriptors and Tox21 assay readouts to predict and rationalise acute toxicity. Journal of Cheminformatics, 2019, 11, 36.	6.4	7
60	Traditional Chinese Medicine Herbal Drugs: From Heritage to Future Developments. AAPS Advances in the Pharmaceutical Sciences Series, 2019, , 59-77.	0.0	4
61	Synthesis of C C, C N coupled novel substituted dibutyl benzothiazepinone derivatives and evaluation of their thrombin inhibitory activity. Bioorganic Chemistry, 2019, 87, 142-154.	4.2	6
62	Characterizing ABC-Transporter Substrate-Likeness Using a Clean-Slate Genetic Background. Frontiers in Pharmacology, 2019, 10, 448.	3.6	1
63	Prediction of UGT-mediated Metabolism Using the Manually Curated MetaQSAR Database. ACS Medicinal Chemistry Letters, 2019, 10, 633-638.	3.1	11
64	Regulating Short-time Wind Power Fluctuation by Variable Speed Pumped Storage Unit. , 2019, , .		0
65	Bioinformatic Approaches in the Understanding of Mechanism of Action (<scp>MoA</scp>). Methods and Principles in Medicinal Chemistry, 2019, , 323-363.	0.0	5
66	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
67	Two Novel Tri-Aryl Derivatives Attenuate the Invasion-Promoting Effects of Stromal Mesenchymal Stem Cells on Breast Cancer. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 1002-1011.	1.8	1
68	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. Briefings in Bioinformatics, 2018, 19, bbw105.	6.6	18
69	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
70	eMolTox: prediction of molecular toxicity with confidence. Bioinformatics, 2018, 34, 2508-2509.	4.2	48
71	Common Structural and Pharmacophoric Features of mPGES-1 and LTC4S. Future Medicinal Chemistry, 2018, 10, 259-268.	2.4	2
72	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. Bioinformatics, 2018, 34, 1538-1546.	4.2	394

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73	Maximizing gain in high-throughput screening using conformal prediction. Journal of Cheminformatics, 2018, 10, 7.	6.4	16
74	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	5.7	43
75	Measuring customers benefits of click and collect. Journal of Services Marketing, 2018, 32, 430-442.	3.2	53
76	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
77	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
78	Fragment-Based Drug Discovery of Phosphodiesterase Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1415-1424.	6.6	17
79	Filter-and-Convolve: A Cnn Based Multichannel Complex Concatenation Acoustic Model. , 2018, , .		4
80	Systemic neurotransmitter responses to clinically approved and experimental neuropsychiatric drugs. Nature Communications, 2018, 9, 4699.	13.2	14
81	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
82	Information-Derived Mechanistic Hypotheses for Structural Cardiotoxicity. Chemical Research in Toxicology, 2018, 31, 1119-1127.	3.5	5
83	Can the inhibition of cytochrome P450 in aquatic invertebrates due to azole fungicides be estimated with in silico and in vitro models and extrapolated between species?. Aquatic Toxicology, 2018, 201, 11-20.	4.0	13
84	Dehydration-induced physical strains of cellulose microfibrils in plant cell walls. Carbohydrate Polymers, 2018, 197, 337-348.	10.5	36
85	Extending in Silico Protein Target Prediction Models to Include Functional Effects. Frontiers in Pharmacology, 2018, 9, 613.	3.6	5
86	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
87	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
88	A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria. Malaria Journal, 2018, 17, 160.	2.2	20
89	Structure-based design of allosteric calpain-1 inhibitors populating a novel bioactivity space. European Journal of Medicinal Chemistry, 2018, 157, 1264-1275.	5.7	8
90	Prospectively Validated Proteochemometric Models for the Prediction of Small-Molecule Binding to Bromodomain Proteins. Journal of Chemical Information and Modeling, 2018, 58, 1870-1888.	5.7	14

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91	Discovery of a non-toxic [1,2,4]triazolo[1,5-a]pyrimidin-7-one (WS-10) that modulates ABCB1-mediated multidrug resistance (MDR). Bioorganic and Medicinal Chemistry, 2018, 26, 5006-5017.	3.1	18
92	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
93	A Fast and Quantitative Method for Post-translational Modification and Variant Enabled Mapping of Peptides to Genomes. Journal of Visualized Experiments, 2018, , .	0.3	3
94	Developments in toxicogenomics: understanding and predicting compound-induced toxicity from gene expression data. Molecular Omics, 2018, 14, 218-236.	2.8	94
95	Improving Screening Efficiency through Iterative Screening Using Docking and Conformal Prediction. Journal of Chemical Information and Modeling, 2017, 57, 439-444.	5.7	47
96	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
97	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
98	Fragment Profiling Approach to Inhibitors of the Orphan M. tuberculosis P450 CYP144A1. Biochemistry, 2017, 56, 1559-1572.	2.6	5
99	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
100	Clinical predictors for the prognosis of myasthenia gravis. BMC Neurology, 2017, 17, 77.	1.8	70
101	Polypharmacological in Silico Bioactivity Profiling and Experimental Validation Uncovers Sedative-Hypnotic Effects of Approved and Experimental Drugs in Rat. ACS Chemical Biology, 2017, 12, 1593-1602.	3.6	9
102	Diversity selection, screening and quantitative structureâ€“activity relationships of osmolyte-like additive effects on the thermal stability of a monoclonal antibody. European Journal of Pharmaceutical Sciences, 2017, 97, 151-157.	4.1	12
103	Towards the mode of action of Strobilanthes crispus through integrated computational and experimental analyses. Journal of Plant Biochemistry and Biotechnology, 2017, 26, 451-466.	1.7	3
104	Prediction of synergistic drug combinations. Current Opinion in Systems Biology, 2017, 4, 24-28.	2.8	28
105	The Arrest and Synthetic Novel Psychoactive Drug Relationship. Journal of Drug Issues, 2017, 47, 91-103.	1.3	8
106	Prediction of Antibiotic Interactions Using Descriptors Derived from Molecular Structure. Journal of Medicinal Chemistry, 2017, 60, 3902-3912.	6.6	47
107	3D proteochemometrics: using three-dimensional information of proteins and ligands to address aspects of the selectivity of serine proteases. MedChemComm, 2017, 8, 1037-1045.	3.4	8
108	Innovation in Small-Molecule-Druggable Chemical Space: Where are the Initial Modulators of New Targets Published?. Journal of Chemical Information and Modeling, 2017, 57, 2741-2753.	5.7	11

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109	Fast, Quantitative and Variant Enabled Mapping of Peptides to Genomes. Cell Systems, 2017, 5, 152-156.e4.	6.2	10
110	Towards understanding polyol additive effects on the pH shift-induced aggregation of a monoclonal antibody using high throughput screening and quantitative structure-activity modeling. International Journal of Pharmaceutics, 2017, 530, 165-172.	5.4	2
111	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
112	In silico target prediction for elucidating the mode of action of herbicides including prospective validation. Journal of Molecular Graphics and Modelling, 2017, 71, 70-79.	2.5	15
113	Modelling compound cytotoxicity using conformal prediction and PubChem HTS data. Toxicology Research, 2017, 6, 73-80.	2.2	48
114	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
115	Gene expression variations in high-altitude adaptation: a case study of the Asiatic toad (Bufo) Tj ETQq1 1 0.784314 rgBT /Overlock 10	2.7	12
116	Computer-aided design of multi-target ligands at A1R, A2AR and PDE10A, key proteins in neurodegenerative diseases. Journal of Cheminformatics, 2017, 9, 67.	6.4	11
117	Modeling Polypharmacological Profiles by Affinity Fingerprinting. Current Pharmaceutical Design, 2017, 22, 6885-6894.	1.9	2
118	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.2	100
119	Global Mapping of Traditional Chinese Medicine into Bioactivity Space and Pathways Annotation Improves Mechanistic Understanding and Discovers Relationships between Therapeutic Action (Sub)classes. Evidence-based Complementary and Alternative Medicine, 2016, 2016, 1-25.	1.2	9
120	Novel Adamantanyl-Based Thiadiazolyl Pyrazoles Targeting EGFR in Triple-Negative Breast Cancer. ACS Omega, 2016, 1, 1412-1424.	3.6	46
121	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
122	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
123	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
124	Simultaneous Prediction of four ATPâ€binding Cassette Transportersâ€™ Substrates Using Multiâ€label QSAR. Molecular Informatics, 2016, 35, 514-528.	2.7	8
125	Analysis of Differential Efficacy and Affinity of GABA_A (Î±1/Î±2) Selective Modulators. Molecular Pharmaceutics, 2016, 13, 4001-4012.	4.7	3
126	Data-Driven Derivation of an â€œInformer Compound Setâ€•for Improved Selection of Active Compounds in High-Throughput Screening. Journal of Chemical Information and Modeling, 2016, 56, 1622-1630.	5.7	14

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127	Identification of HDAC6â€Selective Inhibitors of Low Cancer Cell Cytotoxicity. ChemMedChem, 2016, 11, 81-92.	3.4	29
128	Designing Irreversible Inhibitorsâ€"Worth the Effort?. ChemMedChem, 2016, 11, 22-30.	3.4	61
129	Using a Human Drug Network for generating novel hypotheses about drugs. Intelligent Data Analysis, 2016, 20, 183-197.	0.9	6
130	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
131	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
132	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
133	Nano-MoO₃-mediated synthesis of bioactive thiazolidin-4-ones acting as anti-bacterial agents and their mode-of-action analysis using in silico target prediction, docking and similarity searching. New Journal of Chemistry, 2016, 40, 2189-2199.	2.7	4
134	ARWAR: A network approach for predicting Adverse Drug Reactions. Computers in Biology and Medicine, 2016, 68, 101-108.	7.3	17
135	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	2.2	11
136	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
137	A multi-label approach to target prediction taking ligand promiscuity into account. Journal of Cheminformatics, 2015, 7, 24.	6.4	31
138	Improved Chemical Structureâ€"Activity Modeling Through Data Augmentation. Journal of Chemical Information and Modeling, 2015, 55, 2682-2692.	5.7	39
139	Using a Human Disease Network for augmenting prior knowledge about diseases. Intelligent Data Analysis, 2015, 19, 897-916.	0.9	3
140	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
141	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
142	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
143	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
144	Synergy Maps: exploring compound combinations using network-based visualization. Journal of Cheminformatics, 2015, 7, 36.	6.4	33

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145	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
146	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
147	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
148	Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262.	5.7	23
149	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. Journal of Cheminformatics, 2015, 7, 1.	6.4	141
150	Identification of the first surrogate agonists for the G protein-coupled receptor GPR132. RSC Advances, 2015, 5, 48551-48557.	3.7	8
151	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
152	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
153	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
154	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
155	Cheminformatics Research at the Unilever Centre for Molecular Science Informatics Cambridge. Molecular Informatics, 2015, 34, 626-633.	2.7	0
156	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. Molecular Informatics, 2015, 34, 357-366.	2.7	27
157	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
158	MOLPRINT 2D-based identification and synthesis of novel chromene based small molecules that target PLA2: validation through chemo- and bioinformatics approaches. RSC Advances, 2015, 5, 89797-89808.	3.7	7
159	Synthesis, characterization and in vitro evaluation of novel enantiomerically-pure sulphonamide antimalarials. Organic and Biomolecular Chemistry, 2015, 13, 10681-10690.	2.9	9
160	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
161	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.4	112
162	In Silico Identification of Irreversible Cathepsin B Inhibitors as Anti- Cancer Agents: Virtual Screening, Covalent Docking Analysis and Molecular Dynamics Simulations. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 399-410.	1.1	6

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163	Novel Benzoxazine-Based Aglycones Block Glucose Uptake In Vivo by Inhibiting Glycosidases. PLoS ONE, 2014, 9, e102759.	2.5	15
164	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
165	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
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