Andreas Bender

List of Publications by Year in Descending Order

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	DDREL: From drug-drug relationships to drug repurposing. *Intelligent Data Analysis*, **2022**, 26, 221-237	1.1	1
280	Computational analyses of mechanism of action (MoA): data, methods and integration.. *RSC Chemical Biology*, **2022**, 3, 170-200	3	4
279	Applications of Artificial Intelligence in Drug Design: Opportunities and Challenges. *Methods in Molecular Biology*, **2022**, 2390, 1-59	1.4	1
278	A systems genomics approach to uncover patient-specific pathogenic pathways and proteins in ulcerative colitis.. *Nature Communications*, **2022**, 13, 2299	17.4	0
277	Machine Learning Models for Human Pharmacokinetic Parameters with In-House Validation. *Molecular Pharmaceutics*, **2021**, 18, 4520-4530	5.6	4
276	Comparison of Chemical Structure and Cell Morphology Information for Multitask Bioactivity Predictions. *Journal of Chemical Information and Modeling*, **2021**, 61, 1444-1456	6.1	8
275	Structure-based identification of dual ligands at the AR and PDE10A with anti-proliferative effects in lung cancer cell-lines. *Journal of Cheminformatics*, **2021**, 13, 17	8.6	1
274	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	2.8	0
273	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	8.8	22
272	Comparison of structure- and ligand-based scoring functions for deep generative models: a GPCR case study. *Journal of Cheminformatics*, **2021**, 13, 39	8.6	9
271	Transcriptional drug repositioning and cheminformatics approach for differentiation therapy of leukaemia cells. *Scientific Reports*, **2021**, 11, 12537	4.9	2
270	Neurochemical underpinning of hemodynamic response to neuropsychiatric drugs: A meta- and cluster analysis of preclinical studies. *Journal of Cerebral Blood Flow and Metabolism*, **2021**, 41, 874-885	7.3	2
269	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	4	3
268	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	4	4
267	Predicting and understanding synergistic pairwise compound combinations of Shexian Baoxin Pill (SBP) using network biology. *Synergy*, **2021**, 11, 100073	0.9	1
266	Drug Combination Modeling **2021**, 269-282		
265	Prediction and mechanistic analysis of drug-induced liver injury (DILI) based on chemical structure. *Biology Direct*, **2021**, 16, 6	7.2	5

264	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	4	5
263	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	5.6	4
262	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	8.8	39
261	Computational drug repositioning for ischemic stroke: neuroprotective drug discovery. *Future Medicinal Chemistry*, **2021**, 13, 1271-1283	4.1	1
260	Probabilistic Random Forest improves bioactivity predictions close to the classification threshold by taking into account experimental uncertainty. *Journal of Cheminformatics*, **2021**, 13, 62	8.6	0
259	Prediction and identification of synergistic compound combinations against pancreatic cancer cells. *IScience*, **2021**, 24, 103080	6.1	1
258	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	3.1	2
257	approaches in organ toxicity hazard assessment: current status and future needs in predicting liver toxicity.. *Computational Toxicology*, **2021**, 20, 100187-100187	3.1	3
256	Establishing GPCR Targets of hMAO Active Anthraquinones from Linn Seeds Using and Methods. *ACS Omega*, **2020**, 5, 7705-7715	3.9	3
255	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	8.6	13
254	QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction. *Journal of Cheminformatics*, **2020**, 12, 41	8.6	7
253	Structural Chemogenomics **2020**, 53-77		1
252	Identification of Intrinsic Drug Resistance and Its Biomarkers in High-Throughput Pharmacogenomic and CRISPR Screens. *Patterns*, **2020**, 1, 100065	5.1	3
251	Comparison of Scaling Methods to Obtain Calibrated Probabilities of Activity for Protein-Ligand Predictions. *Journal of Chemical Information and Modeling*, **2020**, 60, 4546-4559	6.1	4
250	Transcriptomics predicts compound synergy in drug and natural product treated glioblastoma cells. *PLoS ONE*, **2020**, 15, e0239551	3.7	6
249	Understanding Conditional Associations between ToxCast Readouts and the Hepatotoxicity of Compounds Using Rule-Based Methods. *Chemical Research in Toxicology*, **2020**, 33, 137-153	4	2
248	EMDIP: An Entropy Measure to Discover Important Proteins in PPI networks. *Computers in Biology and Medicine*, **2020**, 120, 103740	7	3
247	Sulfated Ceria Catalyzed Synthesis of Imidazopyridines and Their Implementation as DNA Minor Groove Binders. *Chemistry and Biodiversity*, **2019**, 16, e1800435	2.5	2

246	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. *Journal of Cheminformatics*, **2019**, 11, 41	8.6	29
245	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. *Journal of Chemical Information and Modeling*, **2019**, 59, 3330-3339	6.1	18
244	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	8.6	3
243	Traditional Chinese Medicine Herbal Drugs: From Heritage to Future Developments. *AAPS Advances in the Pharmaceutical Sciences Series*, **2019**, 59-77	0.5	1
242	Synthesis of CC, CN coupled novel substituted dibutyl benzothiazepinone derivatives and evaluation of their thrombin inhibitory activity. *Bioorganic Chemistry*, **2019**, 87, 142-154	5.1	2
241	Characterizing ABC-Transporter Substrate-Likeness Using a Clean-Slate Genetic Background. *Frontiers in Pharmacology*, **2019**, 10, 448	5.6	1
240	Triazole-Pyridine Dicarbonitrile Targets Phosphodiesterase 4 to Induce Cytotoxicity in Lung Carcinoma Cells. *Chemistry and Biodiversity*, **2019**, 16, e1900234	2.5	6
239	Applying synergy metrics to combination screening data: agreements, disagreements and pitfalls. *Drug Discovery Today*, **2019**, 24, 2286-2298	8.8	38
238	Elucidating Compound Mechanism of Action and Predicting Cytotoxicity Using Machine Learning Approaches, Taking Prediction Confidence into Account. *Current Protocols in Chemical Biology*, **2019**, 11, e73	1.8	1
237	Prediction of UGT-mediated Metabolism Using the Manually Curated MetaQSAR Database. *ACS Medicinal Chemistry Letters*, **2019**, 10, 633-638	4.3	5
236	Bioinformatic Approaches in the Understanding of Mechanism of Action (MoA). *Methods and Principles in Medicinal Chemistry*, **2019**, 323-363	0.4	2
235	Understanding and predicting disease relationships through similarity fusion. *Bioinformatics*, **2019**, 35, 1213-1220	7.2	5
234	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	6.1	40
233	eMolTox: prediction of molecular toxicity with confidence. *Bioinformatics*, **2018**, 34, 2508-2509	7.2	24
232	Common structural and pharmacophoric features of mPGES-1 and LTC4S. *Future Medicinal Chemistry*, **2018**, 10, 259-268	4.1	1
231	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. *Bioinformatics*, **2018**, 34, 1538-1546	7.2	151
230	Maximizing gain in high-throughput screening using conformal prediction. *Journal of Cheminformatics*, **2018**, 10, 7	8.6	12
229	Conformal Regression for Quantitative Structure-Activity Relationship Modeling-Quantifying Prediction Uncertainty. *Journal of Chemical Information and Modeling*, **2018**, 58, 1132-1140	6.1	27

228	Orthologue chemical space and its influence on target prediction. *Bioinformatics*, **2018**, 34, 72-79	7.2	18
227	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. *Briefings in Bioinformatics*, **2018**, 19, 277-285	13.4	15
226	Extending Protein Target Prediction Models to Include Functional Effects. *Frontiers in Pharmacology*, **2018**, 9, 613	5.6	3
225	Synthesis of Structurally Diverse N-Substituted Quaternary-Carbon-Containing Small Molecules from Disubstituted Propargyl Amino Esters. *Chemistry - A European Journal*, **2018**, 24, 13681-13687	4.8	21
224	A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria. *Malaria Journal*, **2018**, 17, 160	3.6	11
223	Structure-based design of allosteric calpain-1 inhibitors populating a novel bioactivity space. *European Journal of Medicinal Chemistry*, **2018**, 157, 1264-1275	6.8	6
222	Prospectively Validated Proteochemometric Models for the Prediction of Small-Molecule Binding to Bromodomain Proteins. *Journal of Chemical Information and Modeling*, **2018**, 58, 1870-1888	6.1	9
221	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	3.4	10
220	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. *Journal of Chemical Information and Modeling*, **2018**, 58, 2000-2014	6.1	21
219	A Fast and Quantitative Method for Post-translational Modification and Variant Enabled Mapping of Peptides to Genomes. *Journal of Visualized Experiments*, **2018**,	1.6	2
218	Developments in toxicogenomics: understanding and predicting compound-induced toxicity from gene expression data. *Molecular Omics*, **2018**, 14, 218-236	4.4	60
217	Identification of Novel Aurora Kinase A (AURKA) Inhibitors via Hierarchical Ligand-Based Virtual Screening. *Journal of Chemical Information and Modeling*, **2018**, 58, 36-47	6.1	15
216	Fragment-Based Drug Discovery of Phosphodiesterase Inhibitors. *Journal of Medicinal Chemistry*, **2018**, 61, 1415-1424	8.3	14
215	Systemic neurotransmitter responses to clinically approved and experimental neuropsychiatric drugs. *Nature Communications*, **2018**, 9, 4699	17.4	7
214	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	11.5	34
213	Using Machine Learning to Predict Synergistic Antimalarial Compound Combinations With Novel Structures. *Frontiers in Pharmacology*, **2018**, 9, 1096	5.6	18
212	Information-Derived Mechanistic Hypotheses for Structural Cardiotoxicity. *Chemical Research in Toxicology*, **2018**, 31, 1119-1127	4	3
211	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	5.1	9

210	Improving Screening Efficiency through Iterative Screening Using Docking and Conformal Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 439-444	6.1	30
209	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	5	16
208	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	6.1	30
207	Fragment Profiling Approach to Inhibitors of the Orphan M. tuberculosis P450 CYP144A1. *Biochemistry*, **2017**, 56, 1559-1572	3.2	5
206	Concordance analysis of microarray studies identifies representative gene expression changes in Parkinson's disease: a comparison of 33 human and animal studies. *BMC Neurology*, **2017**, 17, 58	3.1	15
205	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	4.9	7
204	Diversity selection, screening and quantitative structure-activity relationships of osmolyte-like additive effects on the thermal stability of a monoclonal antibody. *European Journal of Pharmaceutical Sciences*, **2017**, 97, 151-157	5.1	8
203	Towards the mode of action of Strobilanthes crispus through integrated computational and experimental analyses. *Journal of Plant Biochemistry and Biotechnology*, **2017**, 26, 451-466	1.6	1
202	Prediction of synergistic drug combinations. *Current Opinion in Systems Biology*, **2017**, 4, 24-28	3.2	18
201	Prediction of Antibiotic Interactions Using Descriptors Derived from Molecular Structure. *Journal of Medicinal Chemistry*, **2017**, 60, 3902-3912	8.3	24
200	3D proteochemometrics: using three-dimensional information of proteins and ligands to address aspects of the selectivity of serine proteases. *MedChemComm*, **2017**, 8, 1037-1045	5	5
199	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	6.1	5
198	Computer-aided design of multi-target ligands at AR, AR and PDE10A, key proteins in neurodegenerative diseases. *Journal of Cheminformatics*, **2017**, 9, 67	8.6	10
197	Fast, Quantitative and Variant Enabled Mapping of Peptides to Genomes. *Cell Systems*, **2017**, 5, 152-156.e4	8.6	6
196	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	6.5	2
195	Identification of Novel Class of Triazolo-Thiadiazoles as Potent Inhibitors of Human Heparanase and their Anticancer Activity. *BMC Cancer*, **2017**, 17, 235	4.8	38
194	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	2.8	4
193	Modelling compound cytotoxicity using conformal prediction and PubChem HTS data. *Toxicology Research*, **2017**, 6, 73-80	2.6	40

192	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	5	15
191	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. *Bioinformatics*, **2016**, 32, 85-95	7.2	60
190	Understanding Cytotoxicity and Cytostaticity in a High-Throughput Screening Collection. *ACS Chemical Biology*, **2016**, 11, 3007-3023	4.9	22
189	Using a Human Drug Network for generating novel hypotheses about drugs. *Intelligent Data Analysis*, **2016**, 20, 183-197	1.1	4
188	Synthesis and in vitro evaluation of hydrazinyl phthalazines against malaria parasite, Plasmodium falciparum. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 3300-3306	2.9	25
187	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
186	Adamantyl-tethered-biphenylic compounds induce apoptosis in cancer cells by targeting Bcl homologs. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 1056-1060	2.9	29
185	Analysis of Iterative Screening with Stepwise Compound Selection Based on Novartis In-house HTS Data. *ACS Chemical Biology*, **2016**, 11, 1255-64	4.9	33
184	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	3.6	3
183	ARWAR: A network approach for predicting Adverse Drug Reactions. *Computers in Biology and Medicine*, **2016**, 68, 101-8	7	11
182	Trisubstituted-Imidazoles Induce Apoptosis in Human Breast Cancer Cells by Targeting the Oncogenic PI3K/Akt/mTOR Signaling Pathway. *PLoS ONE*, **2016**, 11, e0153155	3.7	84
181	Modeling Polypharmacological Profiles by Affinity Fingerprinting. *Current Pharmaceutical Design*, **2016**, 22, 6885-6894	3.3	2
180	Current Trends in Drug Sensitivity Prediction. *Current Pharmaceutical Design*, **2016**, 22, 6918-6927	3.3	9
179	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. *Toxicology Research*, **2016**, 5, 883-894	2.6	7
178	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, 2106465	2.3	6
177	Novel Adamantanyl-Based Thiadiazolyl Pyrazoles Targeting EGFR in Triple-Negative Breast Cancer. *ACS Omega*, **2016**, 1, 1412-1424	3.9	34
176	A novel applicability domain technique for mapping predictive reliability across the chemical space of a QSAR: reliability-density neighbourhood. *Journal of Cheminformatics*, **2016**, 8,	8.6	21
175	Nano-cuprous oxide catalyzed one-pot synthesis of a carbazole-based STAT3 inhibitor: a facile approach via intramolecular C–N bond formation reactions. *RSC Advances*, **2016**, 6, 36775-36785	3.7	15

174	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. *Drug Discovery Today*, **2016**, 21, 225-38	8.8	108
173	Simultaneous Prediction of four ATP-binding Cassette Transporters' Substrates Using Multi-label QSAR. *Molecular Informatics*, **2016**, 35, 514-528	3.8	6
172	Analysis of Differential Efficacy and Affinity of GABA (A1/2) Selective Modulators. *Molecular Pharmaceutics*, **2016**, 13, 4001-4012	5.6	2
171	Data-Driven Derivation of an "Informer Compound Set" for Improved Selection of Active Compounds in High-Throughput Screening. *Journal of Chemical Information and Modeling*, **2016**, 56, 1622-30	6.1	13
170	How Consistent are Publicly Reported Cytotoxicity Data? Large-Scale Statistical Analysis of the Concordance of Public Independent Cytotoxicity Measurements. *ChemMedChem*, **2016**, 11, 57-71	3.7	19
169	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. *Journal of Cheminformatics*, **2015**, 7, 1	8.6	70
168	Identification of the first surrogate agonists for the G protein-coupled receptor GPR132. *RSC Advances*, **2015**, 5, 48551-48557	3.7	7
167	Design, synthesis and evaluation of semi-synthetic triazole-containing caffeic acid analogues as 5-lipoxygenase inhibitors. *European Journal of Medicinal Chemistry*, **2015**, 101, 573-83	6.8	21
166	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, 6157-65	3.4	74
165	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, 9381-7	3.9	36
164	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	8.6	26
163	Cheminformatics Research at the Unilever Centre for Molecular Science Informatics Cambridge. *Molecular Informatics*, **2015**, 34, 626-633	3.8	
162	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. *Molecular Informatics*, **2015**, 34, 357-66	3.8	20
161	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. *Journal of Cheminformatics*, **2015**, 7, 45	8.6	31
160	Target prediction utilising negative bioactivity data covering large chemical space. *Journal of Cheminformatics*, **2015**, 7, 51	8.6	76
159	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	4
158	Synthesis, characterization and in vitro evaluation of novel enantiomerically-pure sulphonamide antimalarials. *Organic and Biomolecular Chemistry*, **2015**, 13, 10681-90	3.9	6
157	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		22

156	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. *MedChemComm*, **2015**, 6, 24-50	5	74
155	A multi-label approach to target prediction taking ligand promiscuity into account. *Journal of Cheminformatics*, **2015**, 7, 24	8.6	23
154	Development of Novel Triazolo-Thiadiazoles from Heterogeneous "Green" Catalysis as Protein Tyrosine Phosphatase 1B Inhibitors. *Scientific Reports*, **2015**, 5, 14195	4.9	32
153	Improved Chemical Structure-Activity Modeling Through Data Augmentation. *Journal of Chemical Information and Modeling*, **2015**, 55, 2682-92	6.1	23
152	Applications of proteochemometrics - from species extrapolation to cell line sensitivity modelling. *BMC Bioinformatics*, **2015**, 16,	3.6	3
151	Using a Human Disease Network for augmenting prior knowledge about diseases. *Intelligent Data Analysis*, **2015**, 19, 897-916	1.1	2
150	A One Pot Synthesis of Novel Bioactive Tri-Substitute-Condensed-Imidazopyridines that Targets Snake Venom Phospholipase A2. *PLoS ONE*, **2015**, 10, e0131896	3.7	24
149	A Nano-MgO and Ionic Liquid-Catalyzed 'Green' Synthesis Protocol for the Development of Adamantyl-Imidazolo-Thiadiazoles as Anti-Tuberculosis Agents Targeting Sterol 14□Demethylase (CYP51). *PLoS ONE*, **2015**, 10, e0139798	3.7	17
148	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, 1413-25	6.1	21
147	Synthesis and characterization of novel oxazines and demonstration that they specifically target cyclooxygenase 2. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 2931-6	2.9	32
146	Synergy Maps: exploring compound combinations using network-based visualization. *Journal of Cheminformatics*, **2015**, 7, 36	8.6	27
145	Metrabase: a cheminformatics and bioinformatics database for small molecule transporter data analysis and (Q)SAR modeling. *Journal of Cheminformatics*, **2015**, 7, 31	8.6	27
144	Using transcriptomics to guide lead optimization in drug discovery projects: Lessons learned from the QSTAR project. *Drug Discovery Today*, **2015**, 20, 505-13	8.8	60
143	Microwave-assisted synthesis, characterization and cytotoxic studies of novel estrogen receptor □ ligands towards human breast cancer cells. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 1804-1807	2.9	27
142	Analyzing multitarget activity landscapes using protein-ligand interaction fingerprints: interaction cliffs. *Journal of Chemical Information and Modeling*, **2015**, 55, 251-62	6.1	22
141	Novel synthetic coumarins that targets NF-□B in Hepatocellular carcinoma. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 893-7	2.9	52
140	Comparing global and local likelihood score thresholds in multiclass laplacian-modified Naive Bayes protein target prediction. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 323-30	1.3	6
139	How diverse are diversity assessment methods? A comparative analysis and benchmarking of molecular descriptor space. *Journal of Chemical Information and Modeling*, **2014**, 54, 230-42	6.1	53

138	A community computational challenge to predict the activity of pairs of compounds. *Nature Biotechnology*, **2014**, 32, 1213-22	44.5	184
137	Novel synthetic biscoumarins target tumor necrosis factor-□n hepatocellular carcinoma in vitro and in vivo. *Journal of Biological Chemistry*, **2014**, 289, 31879-31890	5.4	54
136	Synthesis and biological evaluation of tetrahydropyridinepyrazoles (□FPs)□as inhibitors of STAT3 phosphorylation. *MedChemComm*, **2014**, 5, 32	5	5
135	Synthesis, biological evaluation and in silico and in vitro mode-of-action analysis of novel dihydropyrimidones targeting PPAR-□*RSC Advances*, **2014**, 4, 45143-45146	3.7	24
134	Comparative mode-of-action analysis following manual and automated phenotype detection in Xenopus laevis. *MedChemComm*, **2014**, 5, 386-396	5	2
133	Predicting Toxic Effects of Metabolites. *Methods and Principles in Medicinal Chemistry*, **2014**, 397-412	0.4	1
132	Towards predictive resistance models for agrochemicals by combining chemical and protein similarity via proteochemometric modelling. *Journal of Chemical Biology*, **2014**, 7, 119-23		2
131	A community effort to assess and improve drug sensitivity prediction algorithms. *Nature Biotechnology*, **2014**, 32, 1202-12	44.5	447
130	Novel benzoxazine-based aglycones block glucose uptake in vivo by inhibiting glycosidases. *PLoS ONE*, **2014**, 9, e102759	3.7	14
129	Synthesis and characterization of novel 2-amino-chromene-nitriles that target Bcl-2 in acute myeloid leukemia cell lines. *PLoS ONE*, **2014**, 9, e107118	3.7	46
128	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, 34296-307	5.4	111
127	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. *Future Medicinal Chemistry*, **2014**, 6, 2029-56	4.1	16
126	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, 1023-33	3.7	23
125	Proteochemometric modeling in a Bayesian framework. *Journal of Cheminformatics*, **2014**, 6, 35	8.6	32
124	Biofragments: an approach towards predicting protein function using biologically related fragments and its application to Mycobacterium tuberculosis CYP126. *ChemBioChem*, **2014**, 15, 549-55	3.8	6
123	Relating GPCRs pharmacological space based on ligands chemical similarities. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
122	Using machine learning techniques for rationalising phenotypic readouts from a rat sleeping model. *Journal of Cheminformatics*, **2013**, 5,	8.6	1
121	Annotating targets with pathways: extending approaches to mode of action analysis. *Journal of Cheminformatics*, **2013**, 5,	8.6	1

120	In silico target prediction: identification of on- and off-targets for crop protection agents. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
119	In silico target predictions: defining a benchmarking data set and comparison of performance of the multiclass Naïve Bayes and Parzen-Rosenblatt window. *Journal of Chemical Information and Modeling*, **2013**, 53, 1957-66	6.1	115
118	Experimental confirmation of new drug-target interactions predicted by Drug Profile Matching. *Journal of Medicinal Chemistry*, **2013**, 56, 8377-88	8.3	13
117	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. *Journal of Cheminformatics*, **2013**, 5, 42	8.6	48
116	Benchmarking of protein descriptor sets in proteochemometric modeling (part 1): comparative study of 13 amino acid descriptor sets. *Journal of Cheminformatics*, **2013**, 5, 41	8.6	58
115	Extensions to In Silico Bioactivity Predictions Using Pathway Annotations and Differential Pharmacology Analysis: Application to Xenopus laevis Phenotypic Readouts. *Molecular Informatics*, **2013**, 32, 1009-24	3.8	12
114	Computer-aided (in silico) approaches in the mode-of-action analysis and safety assessment of ostarine and 4-methylamphetamine. *Human Psychopharmacology*, **2013**, 28, 365-78	2.3	1
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