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List of Publications by Year
in descending order

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106	2,948	147801	214800
papers	citations	31 h-index	47 g-index

133	133	133	4404
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	6.1	275
2	Deep Learning in Image Cytometry: A Review. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2019, 95, 366-380.	1.5	145
3	Transfer Learning with Deep Convolutional Neural Networks for Classifying Cellular Morphological Changes. SLAS Discovery, 2019, 24, 466-475.	2.7	115
4	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	2.6	111
5	Towards reproducible computational drug discovery. Journal of Cheminformatics, 2020, 12, 9.	6.1	100
6	The ChEMBL database as linked open data. Journal of Cheminformatics, 2013, 5, 23.	6.1	96
7	Proteochemometric modeling of HIV protease susceptibility. BMC Bioinformatics, 2008, 9, 181.	2.6	70
8	Lessons learned from implementing a national infrastructure in Sweden for storage and analysis of next-generation sequencing data. GigaScience, 2013, 2, 9.	6.4	67
9	Use of historic metabolic biotransformation data as a means of anticipating metabolic sites using MetaPrint2D and Bioclipse. BMC Bioinformatics, 2010, 11, 362.	2.6	66
10	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	6.1	63
11	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	6.4	60
12	WhichCyp: prediction of cytochromes P450 inhibition. Bioinformatics, 2013, 29, 2051-2052.	4.1	57
13	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	2.6	52
14	Experiences with workflows for automating data-intensive bioinformatics. Biology Direct, 2015, 10, 43.	4.6	52
15	Evaluating parameters for ligand-based modeling with random forest on sparse data sets. Journal of Cheminformatics, 2018, 10, 49.	6.1	46
16	Metabolomics: The Stethoscope for the Twenty-First Century. Medical Principles and Practice, 2021, 30, 301-310.	2.4	46
17	Predicting With Confidence: Using Conformal Prediction in Drug Discovery. Journal of Pharmaceutical Sciences, 2021, 110, 42-49.	3.3	46
18	A Unified Proteochemometric Model for Prediction of Inhibition of Cytochrome P450 Isoforms. PLoS ONE, 2013, 8, e66566.	2.5	42

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19	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. BMC Bioinformatics, 2009, 10, 279.	2.6	40
20	Ligand-Based Target Prediction with Signature Fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-2653.	5.4	40
21	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. Journal of Cheminformatics, 2010, 2, 5.	6.1	39
22	Integration of magnetic resonance imaging and protein and metabolite CSF measurements to enable early diagnosis of secondary progressive multiple sclerosis. Theranostics, 2018, 8, 4477-4490.	10.0	39
23	A confidence predictor for logD using conformal regression and a support-vector machine. Journal of Cheminformatics, 2018, 10, 17.	6.1	37
24	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	5.4	35
25	Container-based bioinformatics with Pachyderm. Bioinformatics, 2019, 35, 839-846.	4.1	35
26	Biochemical Differences in Cerebrospinal Fluid between Secondary Progressive and Relapsingâ€“Remitting Multiple Sclerosis. Cells, 2019, 8, 84.	4.1	35
27	The LCB Data Warehouse. Bioinformatics, 2006, 22, 1024-1026.	4.1	34
28	Benchmarking Study of Parameter Variation When Using Signature Fingerprints Together with Support Vector Machines. Journal of Chemical Information and Modeling, 2014, 54, 3211-3217.	5.4	34
29	Large-scale ligand-based predictive modelling using support vector machines. Journal of Cheminformatics, 2016, 8, 39.	6.1	34
30	Toxicology ontology perspectives. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 139-156.	1.5	33
31	Integrated Decision Support for Assessing Chemical Liabilities. Journal of Chemical Information and Modeling, 2011, 51, 1840-1847.	5.4	31
32	Alterations in the tyrosine and phenylalanine pathways revealed by biochemical profiling in cerebrospinal fluid of Huntingtonâ€™s disease subjects. Scientific Reports, 2019, 9, 4129.	3.3	30
33	Advances in Predictions of Oral Bioavailability of Candidate Drugs in Man with New Machine Learning Methodology. Molecules, 2021, 26, 2572.	3.8	30
34	Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of â€˜Omicsâ€™ Data from Human Cell Cultures. ATLA Alternatives To Laboratory Animals, 2015, 43, 325-332.	1.0	29
35	Towards Predicting the Cytochrome P450 Modulation: From QSAR to Proteochemometric Modeling. Current Drug Metabolism, 2017, 18, 540-555.	1.2	28
36	Harmonising and linking biomedical and clinical data across disparate data archives to enable integrative cross-biobank research. European Journal of Human Genetics, 2016, 24, 521-528.	2.8	27

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37	Towards agile large-scale predictive modelling in drug discovery with flow-based programming design principles. Journal of Cheminformatics, 2016, 8, 67.	6.1	26
38	Mass spectrometry based metabolomics for in vitro systems pharmacology: pitfalls, challenges, and computational solutions. Metabolomics, 2017, 13, 79.	3.0	25
39	Proteochemometric Modeling of the Susceptibility of Mutated Variants of the HIV-1 Virus to Reverse Transcriptase Inhibitors. PLoS ONE, 2010, 5, e14353.	2.5	25
40	Linking the Resource Description Framework to cheminformatics and proteochemometrics. Journal of Biomedical Semantics, 2011, 2, S6.	1.6	24
41	Efficient iterative virtual screening with Apache Spark and conformal prediction. Journal of Cheminformatics, 2018, 10, 8.	6.1	24
42	Cancer Biology, Toxicology and Alternative Methods Development Go Handâ€inâ€Hand. Basic and Clinical Pharmacology and Toxicology, 2014, 115, 50-58.	2.5	22
43	SciPipe: A workflow library for agile development of complex and dynamic bioinformatics pipelines. GigaScience, 2019, 8, .	6.4	22
44	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	4.1	22
45	A toxicology ontology roadmap. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 129-137.	1.5	22
46	Predicting Off-Target Binding Profiles With Confidence Using Conformal Prediction. Frontiers in Pharmacology, 2018, 9, 1256.	3.5	21
47	Recommendations on e-infrastructures for next-generation sequencing. GigaScience, 2016, 5, 26.	6.4	19
48	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	19
49	SNIC Science Cloud (SSC): A National-Scale Cloud Infrastructure for Swedish Academia. , 2017, , .		18
50	Deep Learning With Conformal Prediction for Hierarchical Analysis of Large-Scale Whole-Slide Tissue Images. IEEE Journal of Biomedical and Health Informatics, 2021, 25, 371-380.	6.3	18
51	scConnect: a method for exploratory analysis of cellâ€“cell communication based on single-cell RNA-sequencing data. Bioinformatics, 2021, 37, 3501-3508.	4.1	18
52	Deep-learning models for lipid nanoparticle-based drug delivery. Nanomedicine, 2021, 16, 1097-1110.	3.3	18
53	Comparison between lab variability andin silicoprediction errors for the unbound fraction of drugs in human plasma. Xenobiotica, 2021, 51, 1095-1100.	1.1	18
54	On Mechanisms of Reactive Metabolite Formation from Drugs. Mini-Reviews in Medicinal Chemistry, 2013, 13, 720-729.	2.4	17

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55	Computational toxicology using the OpenTox application programming interface and Bioclipse. BMC Research Notes, 2011, 4, 487.	1.4	16
56	Origin of aromatase inhibitory activity via proteochemometric modeling. PeerJ, 2016, 4, e1979.	2.0	16
57	Large-scale virtual screening on public cloud resources with Apache Spark. Journal of Cheminformatics, 2017, 9, 15.	6.1	16
58	The machine learning life cycle and the cloud: implications for drug discovery. Expert Opinion on Drug Discovery, 2021, 16, 1071-1079.	5.0	16
59	A phenomics approach for antiviral drug discovery. BMC Biology, 2021, 19, 156.	3.8	15
60	A quantitative assessment of the Hadoop framework for analyzing massively parallel DNA sequencing data. GigaScience, 2015, 4, 26.	6.4	14
61	Using Predicted Bioactivity Profiles to Improve Predictive Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2830-2837.	5.4	14
62	XMetDB: an open access database for xenobiotic metabolism. Journal of Cheminformatics, 2016, 8, 47.	6.1	13
63	In silico predictionÂof volume of distribution of drugs in man using conformal prediction performs on par with animal data-based models. Xenobiotica, 2021, 51, 1366-1371.	1.1	13
64	The C1C2: A framework for simultaneous model selection and assessment. BMC Bioinformatics, 2008, 9, 360.	2.6	12
65	Scaling Predictive Modeling in Drug Development with Cloud Computing. Journal of Chemical Information and Modeling, 2015, 55, 19-25.	5.4	12
66	Open Source Drug Discovery with Bioclipse. Current Topics in Medicinal Chemistry, 2012, 12, 1980-1986.	2.1	11
67	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	11
68	On-demand virtual research environments using microservices. PeerJ Computer Science, 2019, 5, e232.	4.5	10
69	BioImg.org: A Catalog of Virtual Machine Images for the Life Sciences. Bioinformatics and Biology Insights, 2015, 9, BBI.S28636.	2.0	9
70	Assessing the calibration in toxicological in vitro models with conformal prediction. Journal of Cheminformatics, 2021, 13, 35.	6.1	9
71	The Impact of Reference Data Selection for the Prediction Accuracy of Intrinsic Hepatic Metabolic Clearance. Journal of Pharmaceutical Sciences, 2022, 111, 2645-2649.	3.3	9
72	Applications of the InChI in cheminformatics with the CDK and Bioclipse. Journal of Cheminformatics, 2013, 5, 14.	6.1	8

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73	Automated QuantMap for rapid quantitative molecular network topology analysis. Bioinformatics, 2013, 29, 2369-2370.	4.1	8
74	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. Bioinformatics, 2013, 29, 286-289.	4.1	8
75	Tracking the NGS revolution: managing life science research on shared high-performance computing clusters. GigaScience, 2018, 7, .	6.4	8
76	Morphological profiling of environmental chemicals enables efficient and untargeted exploration of combination effects. Science of the Total Environment, 2022, 832, 155058.	8.0	8
77	Brunn: An open source laboratory information system for microplates with a graphical plate layout design process. BMC Bioinformatics, 2011, 12, 179.	2.6	7
78	Using Iterative MapReduce for Parallel Virtual Screening. , 2013, , .		7
79	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.9	7
80	MaRe: Processing Big Data with application containers on Apache Spark. GigaScience, 2020, 9, .	6.4	6
81	Privacy-Preservation for Publishing Sample Availability Data with Personal Identifiers. Journal of Medical and Bioengineering, 2015, 4, 117-125.	0.5	6
82	In Silico Predictions of the Gastrointestinal Uptake of Macrocycles in Man Using Conformal Prediction Methodology. Journal of Pharmaceutical Sciences, 2022, 111, 2614-2619.	3.3	6
83	An eScience-Bayes strategy for analyzing omics data. BMC Bioinformatics, 2010, 11, 282.	2.6	5
84	Services for prediction of drug susceptibility for HIV proteases and reverse transcriptases at the HIV drug research centre. Bioinformatics, 2011, 27, 1719-1720.	4.1	5
85	Conformal Prediction in Spark: Large-Scale Machine Learning with Confidence. , 2015, , .		5
86	RDFIO: extending Semantic MediaWiki for interoperable biomedical data management. Journal of Biomedical Semantics, 2017, 8, 35.	1.6	5
87	Novel applications of Machine Learning in cheminformatics. Journal of Cheminformatics, 2018, 10, 46.	6.1	5
88	Interpretation of Conformal Prediction Classification Models. Lecture Notes in Computer Science, 2015, , 323-334.	1.3	5
89	In silico predictions of the human pharmacokinetics/toxicokinetics of 65 chemicals from various classes using conformal prediction methodology. Xenobiotica, 2022, 52, 113-118.	1.1	5
90	HTSeq-Hadoop: Extending HTSeq for Massively Parallel Sequencing Data Analysis Using Hadoop. , 2014, , .		4

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91	E-Science technologies in a workflow for personalized medicine using cancer screening as a case study. Journal of the American Medical Informatics Association: JAMIA, 2017, 24, 950-957.	4.4	4
92	Machine Learning Strategies When Transitioning between Biological Assays. Journal of Chemical Information and Modeling, 2021, 61, 3722-3733.	5.4	4
93	Integrating Statistical and Machine-Learning Approach for Meta-Analysis of Bisphenol A-Exposure Datasets Reveals Effects on Mouse Gene Expression within Pathways of Apoptosis and Cell Survival. International Journal of Molecular Sciences, 2021, 22, 10785.	4.1	4
94	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	1.6	3
95	Predicting target profiles with confidence as a service using docking scores. Journal of Cheminformatics, 2020, 12, .	6.1	2
96	Rapid development of cloud-native intelligent data pipelines for scientific data streams using the HASTE Toolkit. GigaScience, 2021, 10, .	6.4	2
97	Migrating to Long-Read Sequencing for Clinical Routine BCR-ABL1 TKI Resistance Mutation Screening. Cancer Informatics, 2022, 21, 117693512211108.	1.9	2
98	Predicting protein network topology clusters from chemical structure using deep learning. Journal of Cheminformatics, 2022, 14, .	6.1	2
99	Synergy Conformal Prediction for Regression. , 2021, , .		1
100	Approaches for containerized scientific workflows in cloud environments with applications in life science. F1000Research, 0, 10, 513.	1.6	1
101	Interactive predictive toxicology with Bioclipse and OpenTox. , 2012, , 35-61.		0
102	SciPipeâ€"Turning Scientific Workflows into Computer Programs. Computing in Science and Engineering, 2019, 21, 109-113.	1.2	0
103	Synergy conformal prediction applied to large-scale bioactivity datasets and in federated learning. Journal of Cheminformatics, 2021, 13, 77.	6.1	0
104	UPPNEX - A solution for Next Generation Sequencing data management and analysis. EMBnet Journal, 2012, 17, 44.	0.6	0
105	Data Integration between Swedish National Clinical Health Registries and Biobanks Using an Availability System. Lecture Notes in Computer Science, 2014, , 32-40.	1.3	0
106	NGS data management and analysis for hundreds of projects: Experiences from Sweden. EMBnet Journal, 2014, 20, 761.	0.6	0