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List of Publications by Year
in descending order

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106 papers	2,948 citations	168829 31 h-index	242451 47 g-index
133 all docs	133 docs citations	133 times ranked	4930 citing authors

#	Article	IF	Citations
1	In silico predictions of the human pharmacokinetics/toxicokinetics of 65 chemicals from various classes using conformal prediction methodology. Xenobiotica, 2022, 52, 113-118.	0.5	5
2	Morphological profiling of environmental chemicals enables efficient and untargeted exploration of combination effects. Science of the Total Environment, 2022, 832, 155058.	3.9	8
3	In Silico Predictions of the Gastrointestinal Uptake of Macrocycles in Man Using Conformal Prediction Methodology. Journal of Pharmaceutical Sciences, 2022, 111, 2614-2619.	1.6	6
4	Migrating to Long-Read Sequencing for Clinical Routine BCR-ABL1 TKI Resistance Mutation Screening. Cancer Informatics, 2022, 21, 117693512211108.	0.9	2
5	The Impact of Reference Data Selection for the Prediction Accuracy of Intrinsic Hepatic Metabolic Clearance. Journal of Pharmaceutical Sciences, 2022, 111, 2645-2649.	1.6	9
6	Predicting protein network topology clusters from chemical structure using deep learning. Journal of Cheminformatics, 2022, 14, .	2.8	2
7	Metabolomics: The Stethoscope for the Twenty-First Century. Medical Principles and Practice, 2021, 30, 301-310.	1.1	46
8	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.	3.9	18
9	Predicting With Confidence: Using Conformal Prediction in Drug Discovery. Journal of Pharmaceutical Sciences, 2021, 110, 42-49.	1.6	46
10	Synergy Conformal Prediction for Regression. , 2021, , .		1
11	Rapid development of cloud-native intelligent data pipelines for scientific data streams using the HASTE Toolkit. GigaScience, 2021, 10, .	3.3	2
12	Advances in Predictions of Oral Bioavailability of Candidate Drugs in Man with New Machine Learning Methodology. Molecules, 2021, 26, 2572.	1.7	30
13	Assessing the calibration in toxicological in vitro models with conformal prediction. Journal of Cheminformatics, 2021, 13, 35.	2.8	9
14	The machine learning life cycle and the cloud: implications for drug discovery. Expert Opinion on Drug Discovery, 2021, 16, 1071-1079.	2.5	16
15	scConnect: a method for exploratory analysis of cellâ€“cell communication based on single-cell RNA-sequencing data. Bioinformatics, 2021, 37, 3501-3508.	1.8	18
16	Deep-learning models for lipid nanoparticle-based drug delivery. Nanomedicine, 2021, 16, 1097-1110.	1.7	18
17	Machine Learning Strategies When Transitioning between Biological Assays. Journal of Chemical Information and Modeling, 2021, 61, 3722-3733.	2.5	4
18	Comparison between lab variability andin silicoprediction errors for the unbound fraction of drugs in human plasma. Xenobiotica, 2021, 51, 1095-1100.	0.5	18

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19	A phenomics approach for antiviral drug discovery. BMC Biology, 2021, 19, 156.	1.7	15
20	Synergy conformal prediction applied to large-scale bioactivity datasets and in federated learning. Journal of Cheminformatics, 2021, 13, 77.	2.8	0
21	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.	1.8	4
22	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.	0.5	13
23	Predicting target profiles with confidence as a service using docking scores. Journal of Cheminformatics, 2020, 12, .	2.8	2
24	Using Predicted Bioactivity Profiles to Improve Predictive Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2830-2837.	2.5	14
25	MaRe: Processing Big Data with application containers on Apache Spark. GigaScience, 2020, 9, .	3.3	6
26	Towards reproducible computational drug discovery. Journal of Cheminformatics, 2020, 12, 9.	2.8	100
27	Container-based bioinformatics with Pachyderm. Bioinformatics, 2019, 35, 839-846.	1.8	35
28	Transfer Learning with Deep Convolutional Neural Networks for Classifying Cellular Morphological Changes. SLAS Discovery, 2019, 24, 466-475.	1.4	115
29	Biochemical Differences in Cerebrospinal Fluid between Secondary Progressive and Relapsingâ€“Remitting Multiple Sclerosis. Cells, 2019, 8, 84.	1.8	35
30	SciPipeâ€”Turning Scientific Workflows into Computer Programs. Computing in Science and Engineering, 2019, 21, 109-113.	1.2	0
31	SciPipe: A workflow library for agile development of complex and dynamic bioinformatics pipelines. GigaScience, 2019, 8, .	3.3	22
32	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
33	Alterations in the tyrosine and phenylalanine pathways revealed by biochemical profiling in cerebrospinal fluid of Huntingtonâ€™s disease subjects. Scientific Reports, 2019, 9, 4129.	1.6	30
34	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
35	Deep Learning in Image Cytometry: A Review. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2019, 95, 366-380.	1.1	145
36	On-demand virtual research environments using microservices. PeerJ Computer Science, 2019, 5, e232.	2.7	10

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37	Tracking the NGS revolution: managing life science research on shared high-performance computing clusters. GigaScience, 2018, 7, .	3.3	8
38	Efficient iterative virtual screening with Apache Spark and conformal prediction. Journal of Cheminformatics, 2018, 10, 8.	2.8	24
39	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	2.5	35
40	Evaluating parameters for ligand-based modeling with random forest on sparse data sets. Journal of Cheminformatics, 2018, 10, 49.	2.8	46
41	Predicting Off-Target Binding Profiles With Confidence Using Conformal Prediction. Frontiers in Pharmacology, 2018, 9, 1256.	1.6	21
42	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.	4.6	39
43	Novel applications of Machine Learning in cheminformatics. Journal of Cheminformatics, 2018, 10, 46.	2.8	5
44	A confidence predictor for logD using conformal regression and a support-vector machine. Journal of Cheminformatics, 2018, 10, 17.	2.8	37
45	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.	2.2	4
46	Large-scale virtual screening on public cloud resources with Apache Spark. Journal of Cheminformatics, 2017, 9, 15.	2.8	16
47	Mass spectrometry based metabolomics for in vitro systems pharmacology: pitfalls, challenges, and computational solutions. Metabolomics, 2017, 13, 79.	1.4	25
48	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	2.8	275
49	SNIC Science Cloud (SSC): A National-Scale Cloud Infrastructure for Swedish Academia. , 2017, , .		18
50	RDFIO: extending Semantic MediaWiki for interoperable biomedical data management. Journal of Biomedical Semantics, 2017, 8, 35.	0.9	5
51	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
52	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
53	Towards Predicting the Cytochrome P450 Modulation: From QSAR to Proteochemometric Modeling. Current Drug Metabolism, 2017, 18, 540-555.	0.7	28
54	Origin of aromatase inhibitory activity via proteochemometric modeling. PeerJ, 2016, 4, e1979.	0.9	16

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55	Towards agile large-scale predictive modelling in drug discovery with flow-based programming design principles. Journal of Cheminformatics, 2016, 8, 67.	2.8	26
56	Large-scale ligand-based predictive modelling using support vector machines. Journal of Cheminformatics, 2016, 8, 39.	2.8	34
57	XMetDB: an open access database for xenobiotic metabolism. Journal of Cheminformatics, 2016, 8, 47.	2.8	13
58	Recommendations on e-infrastructures for next-generation sequencing. GigaScience, 2016, 5, 26.	3.3	19
59	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.	1.4	27
60	Conformal Prediction in Spark: Large-Scale Machine Learning with Confidence. , 2015, , .		5
61	BioImg.org: A Catalog of Virtual Machine Images for the Life Sciences. Bioinformatics and Biology Insights, 2015, 9, BBI.S28636.	1.0	9
62	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.	0.7	29
63	A quantitative assessment of the Hadoop framework for analyzing massively parallel DNA sequencing data. GigaScience, 2015, 4, 26.	3.3	14
64	Experiences with workflows for automating data-intensive bioinformatics. Biology Direct, 2015, 10, 43.	1.9	52
65	Scaling Predictive Modeling in Drug Development with Cloud Computing. Journal of Chemical Information and Modeling, 2015, 55, 19-25.	2.5	12
66	Interpretation of Conformal Prediction Classification Models. Lecture Notes in Computer Science, 2015, , 323-334.	1.0	5
67	Privacy-Preservation for Publishing Sample Availability Data with Personal Identifiers. Journal of Medical and Bioengineering, 2015, 4, 117-125.	0.5	6
68	Cancer Biology, Toxicology and Alternative Methods Development Go Handâ€inâ€Hand. Basic and Clinical Pharmacology and Toxicology, 2014, 115, 50-58.	1.2	22
69	HTSeq-Hadoop: Extending HTSeq for Massively Parallel Sequencing Data Analysis Using Hadoop. , 2014, , .		4
70	Benchmarking Study of Parameter Variation When Using Signature Fingerprints Together with Support Vector Machines. Journal of Chemical Information and Modeling, 2014, 54, 3211-3217.	2.5	34
71	Ligand-Based Target Prediction with Signature Fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-2653.	2.5	40
72	Data Integration between Swedish National Clinical Health Registries and Biobanks Using an Availability System. Lecture Notes in Computer Science, 2014, , 32-40.	1.0	0

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73	NGS data management and analysis for hundreds of projects: Experiences from Sweden. EMBnet Journal, 2014, 20, 761.	0.2	0
74	The ChEMBL database as linked open data. Journal of Cheminformatics, 2013, 5, 23.	2.8	96
75	Lessons learned from implementing a national infrastructure in Sweden for storage and analysis of next-generation sequencing data. GigaScience, 2013, 2, 9.	3.3	67
76	Using Iterative MapReduce for Parallel Virtual Screening. , 2013, , .		7
77	Applications of the InChI in cheminformatics with the CDK and Bioclipse. Journal of Cheminformatics, 2013, 5, 14.	2.8	8
78	WhichCyp: prediction of cytochromes P450 inhibition. Bioinformatics, 2013, 29, 2051-2052.	1.8	57
79	Automated QuantMap for rapid quantitative molecular network topology analysis. Bioinformatics, 2013, 29, 2369-2370.	1.8	8
80	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. Bioinformatics, 2013, 29, 286-289.	1.8	8
81	A Unified Proteochemometric Model for Prediction of Inhibition of Cytochrome P450 Isoforms. PLoS ONE, 2013, 8, e66566.	1.1	42
82	On Mechanisms of Reactive Metabolite Formation from Drugs. Mini-Reviews in Medicinal Chemistry, 2013, 13, 720-729.	1.1	17
83	Interactive predictive toxicology with Bioclipse and OpenTox. , 2012, , 35-61.		0
84	Open Source Drug Discovery with Bioclipse. Current Topics in Medicinal Chemistry, 2012, 12, 1980-1986.	1.0	11
85	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.4	7
86	A toxicology ontology roadmap. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 129-137.	0.9	22
87	Toxicology ontology perspectives. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 139-156.	0.9	33
88	UPPNEX - A solution for Next Generation Sequencing data management and analysis. EMBnet Journal, 2012, 17, 44.	0.2	0
89	Integrated Decision Support for Assessing Chemical Liabilities. Journal of Chemical Information and Modeling, 2011, 51, 1840-1847.	2.5	31
90	Linking the Resource Description Framework to cheminformatics and proteochemometrics. Journal of Biomedical Semantics, 2011, 2, S6.	0.9	24

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91	Services for prediction of drug susceptibility for HIV proteases and reverse transcriptases at the HIV drug research centre. Bioinformatics, 2011, 27, 1719-1720.	1.8	5
92	Computational toxicology using the OpenTox application programming interface and Bioclipse. BMC Research Notes, 2011, 4, 487.	0.6	16
93	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
94	Brunn: An open source laboratory information system for microplates with a graphical plate layout design process. BMC Bioinformatics, 2011, 12, 179.	1.2	7
95	An eScience-Bayes strategy for analyzing omics data. BMC Bioinformatics, 2010, 11, 282.	1.2	5
96	Use of historic metabolic biotransformation data as a means of anticipating metabolic sites using MetaPrint2D and Bioclipse. BMC Bioinformatics, 2010, 11, 362.	1.2	66
97	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. Journal of Cheminformatics, 2010, 2, 5.	2.8	39
98	Proteochemometric Modeling of the Susceptibility of Mutated Variants of the HIV-1 Virus to Reverse Transcriptase Inhibitors. PLoS ONE, 2010, 5, e14353.	1.1	25
99	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. BMC Bioinformatics, 2009, 10, 279.	1.2	40
100	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	1.2	52
101	Proteochemometric modeling of HIV protease susceptibility. BMC Bioinformatics, 2008, 9, 181.	1.2	70
102	The C1C2: A framework for simultaneous model selection and assessment. BMC Bioinformatics, 2008, 9, 360.	1.2	12
103	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	1.2	111
104	The LCB Data Warehouse. Bioinformatics, 2006, 22, 1024-1026.	1.8	34
105	Approaches for containerized scientific workflows in cloud environments with applications in life science. F1000Research, 0, 10, 513.	0.8	1
106	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3