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List of Publications by Year in descending order

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116194 100535 5,328 90 36 70 citations h-index g-index papers 110 110 110 9987 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Emerging technologies and their impact on regulatory science. Experimental Biology and Medicine, 2022, 247, 1-75.	1.1	22
2	Application of Machine Learning Solutions to Optimize Parameter Prediction to Enhance Automatic NMR Metabolite Profiling. Metabolites, 2022, 12, 283.	1.3	o
3	Networks and Graphs Discovery in Metabolomics Data Analysis and Interpretation. Frontiers in Molecular Biosciences, 2022, 9, 841373.	1.6	35
4	Power of mzRAPP-Based Performance Assessments in MS1-Based Nontargeted Feature Detection. Analytical Chemistry, 2022, 94, 8588-8595.	3.2	3
5	Metabolomics: The Stethoscope for the Twenty-First Century. Medical Principles and Practice, 2021, 30, 301-310.	1.1	46
6	mzRAPP: a tool for reliability assessment of data pre-processing in non-targeted metabolomics. Bioinformatics, 2021, 37, 3678-3680.	1.8	5
7	Information Retrieval Using Machine Learning for Biomarker Curation in the Exposome-Explorer. Frontiers in Research Metrics and Analytics, 2021, 6, 689264.	0.9	2
8	Cross-Platform Evaluation of Commercially Targeted and Untargeted Metabolomics Approaches to Optimize the Investigation of Psychiatric Disease. Metabolites, 2021, 11, 609.	1.3	6
9	A New Pipeline for the Normalization and Pooling of Metabolomics Data. Metabolites, 2021, 11, 631.	1.3	15
10	The ABRF Metabolomics Research Group 2016 Exploratory Study: Investigation of Data Analysis Methods for Untargeted Metabolomics. Metabolites, 2020, 10, 128.	1.3	5
11	The Disruptive 4IR in the Life Sciences: Metabolomics. Lecture Notes in Electrical Engineering, 2020, , 227-256.	0.3	4
12	NMR-based plasma metabolic profiling in patients with unstable angina. Iranian Journal of Basic Medical Sciences, 2020, 23, 311-320.	1.0	2
13	Metabolome Analysis. , 2019, , 396-409.		3
14	Use cases, best practice and reporting standards for metabolomics in regulatory toxicology. Nature Communications, 2019, 10, 3041.	5.8	131
15	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64
16	mzTab-M: A Data Standard for Sharing Quantitative Results in Mass Spectrometry Metabolomics. Analytical Chemistry, 2019, 91, 3302-3310.	3.2	43
17	The Metabolomics Societyâ€"Current State of the Membership and Future Directions. Metabolites, 2019, 9, 89.	1.3	2
18	A Tool to Encourage Minimum Reporting Guideline Uptake for Data Analysis in Metabolomics. Metabolites, 2019, 9, 43.	1.3	19

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19	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
20	Metabolomics in early detection and prognosis of acute coronary syndrome. Clinica Chimica Acta, 2019, 495, 43-53.	0.5	30
21	Exposome-Explorer 2.0: an update incorporating candidate dietary biomarkers and dietary associations with cancer risk. Nucleic Acids Research, 2019, 48, D908-D912.	6.5	31
22	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
23	Progress in Standardization of Metabolic Phenotyping Data. , 2019, , 369-384.		0
24	Measurement Technologies. , 2019, , 35-72.		0
25	rDolphin: a GUI R package for proficient automatic profiling of 1D 1H-NMR spectra of study datasets. Metabolomics, 2018, 14, 24.	1.4	52
26	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. Analytical Chemistry, 2018, 90, 649-656.	3.2	50
27	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	1.8	47
28	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. Metabolites, 2018, 8, 51.	1.3	51
29	Improving sample classification by harnessing the potential of 1H-NMR signal chemical shifts. Scientific Reports, 2018, 8, 11886.	1.6	3
30	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. Metabolomics, 2017, 13, 12.	1.4	69
31	Global open data management in metabolomics. Current Opinion in Chemical Biology, 2017, 36, 58-63.	2.8	39
32	mzML2ISA & amp; nmrML2ISA: generating enriched ISA-Tab metadata files from metabolomics XML data. Bioinformatics, 2017, 33, 2598-2600.	1.8	12
33	Discovering and linking public omics data sets using the Omics Discovery Index. Nature Biotechnology, 2017, 35, 406-409.	9.4	159
34	The Human Proteome Organization–Proteomics Standards Initiative Quality Control Working Group: Making Quality Control More Accessible for Biological Mass Spectrometry. Analytical Chemistry, 2017, 89, 4474-4479.	3.2	22
35	Automated assembly of species metabolomes through data submission into a public repository. GigaScience, 2017, 6, 1-4.	3.3	9
36	Navigating freely-available software tools for metabolomics analysis. Metabolomics, 2017, 13, 106.	1.4	173

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37	Proteomics Standards Initiative: Fifteen Years of Progress and Future Work. Journal of Proteome Research, 2017, 16, 4288-4298.	1.8	87
38	Assessing Public Metabolomics Metadata, Towards Improving Quality. Journal of Integrative Bioinformatics, 2017, 14, .	1.0	13
39	Compliance with minimum information guidelines in public metabolomics repositories. Scientific Data, 2017, 4, 170137.	2.4	61
40	A decade after the metabolomics standards initiative it's time for a revision. Scientific Data, 2017, 4, 170138.	2.4	70
41	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
42	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
43	NMR Spectroscopy of Tissues, 1 H MAS. , 2017, , 254-259.		0
44	Editorial: Metabolome Informatics and Statistics: Current State and Emerging Trends. Frontiers in Bioengineering and Biotechnology, 2016, 4, 63.	2.0	3
45	The Time Is Right to Focus on Model Organism Metabolomes. Metabolites, 2016, 6, 8.	1.3	63
46	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
47	Infection Susceptibility in Gastric Intrinsic Factor (Vitamin B ₁₂)-Defective Mice Is Subject to Maternal Influences. MBio, 2016, 7, .	1.8	8
48	MetaboLights: An Openâ€Access Database Repository for Metabolomics Data. Current Protocols in Bioinformatics, 2016, 53, 14.13.1-14.13.18.	25.8	147
49	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
50	From Databases to Big Data., 2016,, 317-331.		5
51	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. Journal of Proteome Research, 2016, 15, 360-373.	1.8	122
52	Mass spectral databases for LC/MS- and GC/MS-based metabolomics: State of the field and future prospects. TrAC - Trends in Analytical Chemistry, 2016, 78, 23-35.	5.8	404
53	SpeckTackle: JavaScript charts for spectroscopy. Journal of Cheminformatics, 2015, 7, 17.	2.8	10
54	Dolphin 1D: Improving Automation of Targeted Metabolomics in Multi-matrix Datasets of \$\$^1\$\$H-NMR Spectra. Advances in Intelligent Systems and Computing, 2015, , 59-67.	0.5	3

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55	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
56	Metabolomics continues to expand: highlights from the 2015 metabolomics conference. Metabolomics, 2015, 11, 1036-1040.	1.4	14
57	Getting the right answers: understanding metabolomics challenges. Expert Review of Molecular Diagnostics, 2015, 15, 97-109.	1.5	42
58	Standardizing the experimental conditions for using urine in NMR-based metabolomic studies with a particular focus on diagnostic studies: a review. Metabolomics, 2015, 11, 872-894.	1.4	196
59	Embedding standards in metabolomics: the Metabolomics Society data standards task group. Metabolomics, 2015, 11, 782-783.	1.4	13
60	Behavioural and molecular endophenotypes in psychotic disorders reveal heritable abnormalities in glutamatergic neurotransmission. Translational Psychiatry, 2015, 5, e540-e540.	2.4	13
61	Dolphin: a tool for automatic targeted metabolite profiling using 1D and 2D 1H-NMR data. Analytical and Bioanalytical Chemistry, 2014, 406, 7967-7976.	1.9	55
62	Genome-Wide Association Study of Metabolic Traits Reveals Novel Gene-Metabolite-Disease Links. PLoS Genetics, 2014, 10, e1004132.	1.5	86
63	The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience. Molecular and Cellular Proteomics, 2014, 13, 2765-2775.	2.5	130
64	Metabolic differences in ripening of Solanum lycopersicum †Ailsa Craig†and three monogenic mutants. Scientific Data, 2014, 1, 140029.	2.4	12
65	Metabolomics in neuroscience and neurology , 2014, , 20-30.		0
66	Expanding natural product chemistry resources at the EBI. Journal of Cheminformatics, 2013, 5, .	2.8	0
67	Dissemination of metabolomics results: role of MetaboLights and COSMOS. GigaScience, 2013, 2, 8.	3.3	28
68	The role of reporting standards for metabolite annotation and identification in metabolomic studies. GigaScience, 2013, 2, 13.	3.3	333
69	Biomarkers of food intake and metabolite differences between plasma and red blood cell matrices; a human metabolomic profile approach. Molecular BioSystems, 2013, 9, 1411.	2.9	23
70	NMR-based metabolomics in human disease diagnosis: applications, limitations, and recommendations. Metabolomics, 2013, 9, 1048-1072.	1.4	203
71	MetaboLights—an open-access general-purpose repository for metabolomics studies and associated meta-data. Nucleic Acids Research, 2013, 41, D781-D786.	6.5	578
72	The MetaboLights repository: curation challenges in metabolomics. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat029.	1.4	46

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73	Neuroscience and Metabolomics. , 2013, , 220-231.		O
74	MetaboLights: towards a new COSMOS of metabolomics data management. Metabolomics, 2012, 8, 757-760.	1.4	79
75	Metabolomics of human breast cancer: new approaches for tumor typing and biomarker discovery. Genome Medicine, 2012, 4, 37.	3.6	88
76	Remodeling of central metabolism in invasive breast cancer compared to normal breast tissue – a GC-TOFMS based metabolomics study. BMC Genomics, 2012, 13, 334.	1.2	123
77	A metabolomic strategy defines the regulation of lipid content and global metabolism by Δ9 desaturases in Caenorhabditis elegans. BMC Genomics, 2012, 13, 36.	1.2	28
78	The Study of Mammalian Metabolism through NMR-based Metabolomics. Methods in Enzymology, 2011, 500, 337-351.	0.4	15
79	A metabolomic comparison of mouse models of the Neuronal Ceroid Lipofuscinoses. Journal of Biomolecular NMR, 2011, 49, 175-184.	1.6	11
80	A Metadata description of the data in "A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human.". BMC Research Notes, 2011, 4, 272.	0.6	16
81	1H nuclear magnetic resonance spectroscopy characterisation of metabolic phenotypes in the medulloblastoma of the SMO transgenic mice. British Journal of Cancer, 2010, 103, 1297-1304.	2.9	23
82	1 H MAS NMR Spectroscopy of Tissues. , 2010, , 925-930.		1
83	A metabolomic study of the CRND8 transgenic mouse model of Alzheimer's disease. Neurochemistry International, 2010, 56, 937-947.	1.9	131
84	A Metabolomic Study of Brain Tissues from Aged Mice with Low Expression of the Vesicular Monoamine Transporter 2 (VMAT2) Gene. Neurochemical Research, 2008, 33, 292-300.	1.6	23
85	A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human. Physiological Genomics, 2007, 29, 99-108.	1.0	354
86	Metabolomic applications to neuroscience: more challenges than chances?. Expert Review of Proteomics, 2007, 4, 435-437.	1.3	13
87	Metabolomic investigation of CLN6 neuronal ceroid lipofuscinosis in affected South Hampshire sheep. Journal of Neuroscience Research, 2007, 85, 3494-3504.	1.3	24
88	Backbone resonance assignments of the 25kD N-terminal ATPase domain from the Hsp90 chaperone. Journal of Biomolecular NMR, 2002, 23, 327-328.	1.6	19
89	Towards standard, accessible and reproducible Metabolomics , 0, , .		0
90	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3