

Steffen Neumann

List of Publications by Year in descending order

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Version: 2024-02-01

94
papers

16,140
citations

61984

43
h-index

43889

91
g-index

104
all docs

104
docs citations

104
times ranked

20017
citing authors

#	ARTICLE	IF	CITATIONS
1	A cross-platform toolkit for mass spectrometry and proteomics. <i>Nature Biotechnology</i> , 2012, 30, 918-920.	17.5	2,794
2	MassBank: a public repository for sharing mass spectral data for life sciences. <i>Journal of Mass Spectrometry</i> , 2010, 45, 703-714.	1.6	1,831
3	Highly sensitive feature detection for high resolution LC/MS. <i>BMC Bioinformatics</i> , 2008, 9, 504.	2.6	962
4	CAMERA: An Integrated Strategy for Compound Spectra Extraction and Annotation of Liquid Chromatography/Mass Spectrometry Data Sets. <i>Analytical Chemistry</i> , 2012, 84, 283-289.	6.5	930
5	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. <i>Journal of Cheminformatics</i> , 2016, 8, 3.	6.1	665
6	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , 2020, 17, 905-908.	19.0	650
7	MetaboLights – an open-access general-purpose repository for metabolomics studies and associated meta-data. <i>Nucleic Acids Research</i> , 2013, 41, D781-D786.	14.5	578
8	mzML – a Community Standard for Mass Spectrometry Data. <i>Molecular and Cellular Proteomics</i> , 2011, 10, R110.000133.	3.8	555
9	In silico fragmentation for computer assisted identification of metabolite mass spectra. <i>BMC Bioinformatics</i> , 2010, 11, 148.	2.6	541
10	Mass appeal: metabolite identification in mass spectrometry-focused untargeted metabolomics. <i>Metabolomics</i> , 2013, 9, 44-66.	3.0	452
11	Mass spectral databases for LC/MS- and GC/MS-based metabolomics: State of the field and future prospects. <i>TrAC - Trends in Analytical Chemistry</i> , 2016, 78, 23-35.	11.4	404
12	Mass spectrometry-based metabolomics: a guide for annotation, quantification and best reporting practices. <i>Nature Methods</i> , 2021, 18, 747-756.	19.0	403
13	Toward interoperable bioscience data. <i>Nature Genetics</i> , 2012, 44, 121-126.	21.4	362
14	Effect-directed analysis supporting monitoring of aquatic environments – An in-depth overview. <i>Science of the Total Environment</i> , 2016, 544, 1073-1118.	8.0	288
15	IPO: a tool for automated optimization of XCMS parameters. <i>BMC Bioinformatics</i> , 2015, 16, 118.	2.6	249
16	ISA software suite: supporting standards-compliant experimental annotation and enabling curation at the community level. <i>Bioinformatics</i> , 2010, 26, 2354-2356.	4.1	247
17	Future water quality monitoring – Adapting tools to deal with mixtures of pollutants in water resource management. <i>Science of the Total Environment</i> , 2015, 512-513, 540-551.	8.0	243
18	RAMClust: A Novel Feature Clustering Method Enables Spectral-Matching-Based Annotation for Metabolomics Data. <i>Analytical Chemistry</i> , 2014, 86, 6812-6817.	6.5	219

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19	Metabolite identification: are you sure? And how do your peers gauge your confidence?. <i>Metabolomics</i> , 2014, 10, 350-353.	3.0	205
20	MetFusion: integration of compound identification strategies. <i>Journal of Mass Spectrometry</i> , 2013, 48, 291-298.	1.6	163
21	The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. <i>Science of the Total Environment</i> , 2015, 503-504, 22-31.	8.0	163
22	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. <i>Analytical and Bioanalytical Chemistry</i> , 2010, 398, 2779-2788.	3.7	159
23	Critical assessment of alignment procedures for LC-MS proteomics and metabolomics measurements. <i>BMC Bioinformatics</i> , 2008, 9, 375.	2.6	152
24	Natural variation of root exudates in <i>Arabidopsis thaliana</i> -linking metabolomic and genomic data. <i>Scientific Reports</i> , 2016, 6, 29033.	3.3	143
25	COordination of Standards in MetabOlomics (COSMOS): facilitating integrated metabolomics data access. <i>Metabolomics</i> , 2015, 11, 1587-1597.	3.0	140
26	Metabolome Analysis of Biosynthetic Mutants Reveals a Diversity of Metabolic Changes and Allows Identification of a Large Number of New Compounds in <i>Arabidopsis</i> . <i>Plant Physiology</i> , 2008, 147, 2107-2120.	4.8	138
27	The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2765-2775.	3.8	130
28	Critical Assessment of Small Molecule Identification 2016: automated methods. <i>Journal of Cheminformatics</i> , 2017, 9, 22.	6.1	122
29	PredRet: Prediction of Retention Time by Direct Mapping between Multiple Chromatographic Systems. <i>Analytical Chemistry</i> , 2015, 87, 9421-9428.	6.5	121
30	Current Challenges in Plant Eco-Metabolomics. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1385.	4.1	106
31	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. <i>BMC Bioinformatics</i> , 2008, 9, 400.	2.6	97
32	Data standards can boost metabolomics research, and if there is a will, there is a way. <i>Metabolomics</i> , 2016, 12, 14.	3.0	97
33	Discovering Regulated Metabolite Families in Untargeted Metabolomics Studies. <i>Analytical Chemistry</i> , 2016, 88, 8082-8090.	6.5	72
34	Comparative expression profiling reveals a role of the root apoplast in local phosphate response. <i>BMC Plant Biology</i> , 2016, 16, 106.	3.6	70
35	TraML – A Standard Format for Exchange of Selected Reaction Monitoring Transition Lists. <i>Molecular and Cellular Proteomics</i> , 2012, 11, R111.015040.	3.8	65
36	The metaRbolomics Toolbox in Bioconductor and beyond. <i>Metabolites</i> , 2019, 9, 200.	2.9	64

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37	Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. <i>Journal of Cheminformatics</i> , 2021, 13, 19.	6.1	63
38	SPLASH, a hashed identifier for mass spectra. <i>Nature Biotechnology</i> , 2016, 34, 1099-1101.	17.5	61
39	PhenoMeNal: processing and analysis of metabolomics data in the cloud. <i>GigaScience</i> , 2019, 8, .	6.4	60
40	Consensus Structure Elucidation Combining GC/EI-MS, Structure Generation, and Calculated Properties. <i>Analytical Chemistry</i> , 2012, 84, 3287-3295.	6.5	57
41	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. <i>Metabolites</i> , 2018, 8, 51.	2.9	51
42	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. <i>Analytical Chemistry</i> , 2018, 90, 649-656.	6.5	50
43	Bioinformatics can boost metabolomics research. <i>Journal of Biotechnology</i> , 2017, 261, 137-141.	3.8	49
44	Golden Mutagenesis: An efficient multi-site-saturation mutagenesis approach by Golden Gate cloning with automated primer design. <i>Scientific Reports</i> , 2019, 9, 10932.	3.3	48
45	Expanding the Use of Spectral Libraries in Proteomics. <i>Journal of Proteome Research</i> , 2018, 17, 4051-4060.	3.7	47
46	Improving MetFrag with statistical learning of fragment annotations. <i>BMC Bioinformatics</i> , 2019, 20, 376.	2.6	44
47	mzTab-M: A Data Standard for Sharing Quantitative Results in Mass Spectrometry Metabolomics. <i>Analytical Chemistry</i> , 2019, 91, 3302-3310.	6.5	43
48	A Modular and Expandable Ecosystem for Metabolomics Data Annotation in R. <i>Metabolites</i> , 2022, 12, 173.	2.9	43
49	Functional Traits 2.0: The power of the metabolome for ecology. <i>Journal of Ecology</i> , 2022, 110, 4-20.	4.0	42
50	Metabolite profiling and beyond: approaches for the rapid processing and annotation of human blood serum mass spectrometry data. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 5037-5048.	3.7	41
51	The significance of tree-tree interactions for forest ecosystem functioning. <i>Basic and Applied Ecology</i> , 2021, 55, 33-52.	2.7	38
52	Nearline acquisition and processing of liquid chromatography-tandem mass spectrometry data. <i>Metabolomics</i> , 2013, 9, 84-91.	3.0	35
53	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. <i>Metabolites</i> , 2013, 3, 517-538.	2.9	35
54	BiNChE: A web tool and library for chemical enrichment analysis based on the ChEBI ontology. <i>BMC Bioinformatics</i> , 2015, 16, 56.	2.6	35

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55	Networks and Graphs Discovery in Metabolomics Data Analysis and Interpretation. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 841373.	3.5	35
56	Chemical Diversity and Classification of Secondary Metabolites in Nine Bryophyte Species. <i>Metabolites</i> , 2019, 9, 222.	2.9	34
57	Seasonal variation of secondary metabolites in nine different bryophytes. <i>Ecology and Evolution</i> , 2018, 8, 9105-9117.	1.9	33
58	Annotation of LC/ESI-MS Mass Signals. , 2007, , 371-380.		33
59	Meeting Report from the Second "Minimum Information for Biological and Biomedical Investigations" (MIBBI) workshop. <i>Standards in Genomic Sciences</i> , 2010, 3, 259-266.	1.5	32
60	CASMI: And the Winner is . . . <i>Metabolites</i> , 2013, 3, 412-439.	2.9	30
61	Reshaping of the <i>Arabidopsis thaliana</i> Proteome Landscape and Co-regulation of Proteins in Development and Immunity. <i>Molecular Plant</i> , 2020, 13, 1709-1732.	8.3	26
62	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. <i>Research Ideas and Outcomes</i> , 0, 6, .	1.0	25
63	The Risa R/Bioconductor package: integrative data analysis from experimental metadata and back again. <i>BMC Bioinformatics</i> , 2014, 15, S11.	2.6	22
64	Interoperable and scalable data analysis with microservices: applications in metabolomics. <i>Bioinformatics</i> , 2019, 35, 3752-3760.	4.1	22
65	LipidFrag: Improving reliability of in silico fragmentation of lipids and application to the <i>Caenorhabditis elegans</i> lipidome. <i>PLoS ONE</i> , 2017, 12, e0172311.	2.5	21
66	Annotation of metabolites from gas chromatography/atmospheric pressure chemical ionization tandem mass spectrometry data using an in silico generated compound database and MetFrag. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1521-1529.	1.5	20
67	Experiment design beyond gut feeling: statistical tests and power to detect differential metabolites in mass spectrometry data. <i>Metabolomics</i> , 2015, 11, 851-860.	3.0	20
68	Plant-to-Plant Variability in Root Metabolite Profiles of 19 <i>Arabidopsis thaliana</i> Accessions Is Substance-Class-Dependent. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1565.	4.1	20
69	Tree species richness differentially affects the chemical composition of leaves, roots and root exudates in four subtropical tree species. <i>Journal of Ecology</i> , 2022, 110, 97-116.	4.0	20
70	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	1.6	19
71	Prediction, Detection, and Validation of Isotope Clusters in Mass Spectrometry Data. <i>Metabolites</i> , 2016, 6, 37.	2.9	18
72	Computational annotation of plant metabolomics profiles via a novel network-assisted approach. <i>Metabolomics</i> , 2013, 9, 904-918.	3.0	17

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73	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. <i>Mass Spectrometry</i> , 2014, 3, S0036-S0036.	0.6	16
74	ChemFrag: Chemically meaningful annotation of fragment ion mass spectra. <i>Journal of Mass Spectrometry</i> , 2018, 53, 1104-1115.	1.6	14
75	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 4683-4700.	3.7	14
76	Embedding standards in metabolomics: the Metabolomics Society data standards task group. <i>Metabolomics</i> , 2015, 11, 782-783.	3.0	13
77	Ontologies4Chem: the landscape of ontologies in chemistry. <i>Pure and Applied Chemistry</i> , 2022, 94, 605-622.	1.9	13
78	Computational workflow to study the seasonal variation of secondary metabolites in nine different bryophytes. <i>Scientific Data</i> , 2018, 5, 180179.	5.3	12
79	Untargeted In Silico Compound Classification—A Novel Metabolomics Method to Assess the Chemodiversity in Bryophytes. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3251.	4.1	11
80	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	1.6	11
81	LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods. <i>Scientific Data</i> , 2021, 8, 52.	5.3	10
82	Modulation of Phosphate Deficiency-Induced Metabolic Changes by Iron Availability in <i>Arabidopsis thaliana</i> . <i>International Journal of Molecular Sciences</i> , 2021, 22, 7609.	4.1	10
83	Database supported candidate search for Metabolite identification. <i>Journal of Integrative Bioinformatics</i> , 2011, 8, 23-38.	1.5	9
84	Tackling CASMI 2012: Solutions from MetFrag and MetFusion. <i>Metabolites</i> , 2013, 3, 623-636.	2.9	8
85	Database supported candidate search for metabolite identification. <i>Journal of Integrative Bioinformatics</i> , 2011, 8, 157.	1.5	7
86	Metabolic drift in the aging nervous system is reflected in human cerebrospinal fluid. <i>Scientific Reports</i> , 2021, 11, 18822.	3.3	6
87	MetHouse: Raw and Preprocessed Mass Spectrometry Data. <i>Journal of Integrative Bioinformatics</i> , 2007, 4, 107-114.	1.5	5
88	Impact of in vitro hormone treatments on the bibenzyl production of <i>Radula complanata</i> . <i>Botany</i> , 0, , .	1.0	5
89	Data format standards in analytical chemistry. <i>Pure and Applied Chemistry</i> , 2022, 94, 725-736.	1.9	4
90	ELIXIR and Toxicology: a community in development. <i>F1000Research</i> , 0, 10, 1129.	1.6	3

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91	Comparing bound and unbound protein structures using energy calculation and rotamer statistics. In <i>Silico Biology</i> , 2002, 2, 351-68.	0.9	3
92	Joint Analysis of Dependent Features within Compound Spectra Can Improve Detection of Differential Features. <i>Frontiers in Bioengineering and Biotechnology</i> , 2015, 3, 129.	4.1	2
93	Fast Approximate Duplicate Detection for 2D-NMR Spectra. , 2007, , 139-155.		2
94	Database driven test case generation for protein-protein docking. <i>Bioinformatics</i> , 2005, 21, 683-684.	4.1	1