Steffen Neumann

List of Publications by Year
in descending order

94 papers	16,140 citations	61857 43 h-index	43802 91 g-index
104 all docs	104 docs citations	104 times ranked	20017 citing authors

#	Article	IF	Citations
1	Tree species richness differentially affects the chemical composition of leaves, roots and root exudates in four subtropical tree species. Journal of Ecology, 2022, 110, 97-116.	1.9	20
2	Functional Traits 2.0: The power of the metabolome for ecology. Journal of Ecology, 2022, 110, 4-20.	1.9	42
3	A Modular and Expandable Ecosystem for Metabolomics Data Annotation in R. Metabolites, 2022, 12, 173.	1.3	43
4	Ontologies4Chem: the landscape of ontologies in chemistry. Pure and Applied Chemistry, 2022, 94, 605-622.	0.9	13
5	Networks and Graphs Discovery in Metabolomics Data Analysis and Interpretation. Frontiers in Molecular Biosciences, 2022, 9, 841373.	1.6	35
6	Data format standards in analytical chemistry. Pure and Applied Chemistry, 2022, 94, 725-736.	0.9	4
7	LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods. Scientific Data, 2021, 8, 52.	2.4	10
8	Untargeted In Silico Compound Classificationâ€"A Novel Metabolomics Method to Assess the Chemodiversity in Bryophytes. International Journal of Molecular Sciences, 2021, 22, 3251.	1.8	11
9	Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. Journal of Cheminformatics, 2021, 13, 19.	2.8	63
10	Mass spectrometry-based metabolomics: a guide for annotation, quantification and best reporting practices. Nature Methods, 2021, 18, 747-756.	9.0	403
11	Modulation of Phosphate Deficiency-Induced Metabolic Changes by Iron Availability in Arabidopsis thaliana. International Journal of Molecular Sciences, 2021, 22, 7609.	1.8	10
12	The significance of tree-tree interactions for forest ecosystem functioning. Basic and Applied Ecology, 2021, 55, 33-52.	1.2	38
13	Metabolic drift in the aging nervous system is reflected in human cerebrospinal fluid. Scientific Reports, 2021, 11, 18822.	1.6	6
14	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	9.0	650
15	Reshaping of the Arabidopsis thaliana Proteome Landscape and Co-regulation of Proteins in Development and Immunity. Molecular Plant, 2020, 13, 1709-1732.	3.9	26
16	Golden Mutagenesis: An efficient multi-site-saturation mutagenesis approach by Golden Gate cloning with automated primer design. Scientific Reports, 2019, 9, 10932.	1.6	48
17	Improving MetFrag with statistical learning of fragment annotations. BMC Bioinformatics, 2019, 20, 376.	1.2	44
18	Chemical Diversity and Classification of Secondary Metabolites in Nine Bryophyte Species. Metabolites, 2019, 9, 222.	1.3	34

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19	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64
20	mzTab-M: A Data Standard for Sharing Quantitative Results in Mass Spectrometry Metabolomics. Analytical Chemistry, 2019, 91, 3302-3310.	3.2	43
21	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. Analytical and Bioanalytical Chemistry, 2019, 411, 4683-4700.	1.9	14
22	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
23	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
24	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
25	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	1.8	47
26	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. Metabolites, 2018, 8, 51.	1.3	51
27	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	1.8	106
28	ChemFrag: Chemically meaningful annotation of fragment ion mass spectra. Journal of Mass Spectrometry, 2018, 53, 1104-1115.	0.7	14
29	Seasonal variation of secondary metabolites in nine different bryophytes. Ecology and Evolution, 2018, 8, 9105-9117.	0.8	33
30	Computational workflow to study the seasonal variation of secondary metabolites in nine different bryophytes. Scientific Data, 2018, 5, 180179.	2.4	12
31	Bioinformatics can boost metabolomics research. Journal of Biotechnology, 2017, 261, 137-141.	1.9	49
32	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	2.8	122
33	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
34	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
35	LipidFrag: Improving reliability of in silico fragmentation of lipids and application to the Caenorhabditis elegans lipidome. PLoS ONE, 2017, 12, e0172311.	1.1	21
36	Plant-to-Plant Variability in Root Metabolite Profiles of 19 Arabidopsis thaliana Accessions Is Substance-Class-Dependent. International Journal of Molecular Sciences, 2016, 17, 1565.	1.8	20

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37	Prediction, Detection, and Validation of Isotope Clusters in Mass Spectrometry Data. Metabolites, 2016, 6, 37.	1.3	18
38	Natural variation of root exudates in Arabidopsis thaliana-linking metabolomic and genomic data. Scientific Reports, 2016, 6, 29033.	1.6	143
39	Comparative expression profiling reveals a role of the root apoplast in local phosphate response. BMC Plant Biology, 2016, 16, 106.	1.6	70
40	Discovering Regulated Metabolite Families in Untargeted Metabolomics Studies. Analytical Chemistry, 2016, 88, 8082-8090.	3.2	72
41	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
42	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. Journal of Cheminformatics, 2016, 8, 3.	2.8	665
43	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
44	Effect-directed analysis supporting monitoring of aquatic environments â€" An in-depth overview. Science of the Total Environment, 2016, 544, 1073-1118.	3.9	288
45	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
46	Annotation of metabolites from gas chromatography/atmospheric pressure chemical ionization tandem mass spectrometry data using an in silico generated compound database and MetFrag. Rapid Communications in Mass Spectrometry, 2015, 29, 1521-1529.	0.7	20
47	Joint Analysis of Dependent Features within Compound Spectra Can Improve Detection of Differential Features. Frontiers in Bioengineering and Biotechnology, 2015, 3, 129.	2.0	2
48	IPO: a tool for automated optimization of XCMS parameters. BMC Bioinformatics, 2015, 16, 118.	1.2	249
49	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
50	Future water quality monitoring â€" Adapting tools to deal with mixtures of pollutants in water resource management. Science of the Total Environment, 2015, 512-513, 540-551.	3.9	243
51	Experiment design beyond gut feeling: statistical tests and power to detect differential metabolites in mass spectrometry data. Metabolomics, 2015, 11, 851-860.	1.4	20
52	BiNChE: A web tool and library for chemical enrichment analysis based on the ChEBI ontology. BMC Bioinformatics, 2015, 16, 56.	1.2	35
53	Embedding standards in metabolomics: the Metabolomics Society data standards task group. Metabolomics, 2015, 11, 782-783.	1.4	13
54	PredRet: Prediction of Retention Time by Direct Mapping between Multiple Chromatographic Systems. Analytical Chemistry, 2015, 87, 9421-9428.	3.2	121

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55	The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. Science of the Total Environment, 2015, 503-504, 22-31.	3.9	163
56	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. Mass Spectrometry, 2014, 3, S0036-S0036.	0.2	16
57	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
58	The Risa R/Bioconductor package: integrative data analysis from experimental metadata and back again. BMC Bioinformatics, 2014, 15, S11.	1.2	22
59	Metabolite identification: are you sure? And how do your peers gauge your confidence?. Metabolomics, 2014, 10, 350-353.	1.4	205
60	RAMClust: A Novel Feature Clustering Method Enables Spectral-Matching-Based Annotation for Metabolomics Data. Analytical Chemistry, 2014, 86, 6812-6817.	3.2	219
61	Metabolite profiling and beyond: approaches for the rapid processing and annotation of human blood serum mass spectrometry data. Analytical and Bioanalytical Chemistry, 2013, 405, 5037-5048.	1.9	41
62	Computational annotation of plant metabolomics profiles via a novel network-assisted approach. Metabolomics, 2013, 9, 904-918.	1.4	17
63	Mass appeal: metabolite identification in mass spectrometry-focused untargeted metabolomics. Metabolomics, 2013, 9, 44-66.	1.4	452
64	Nearline acquisition and processing of liquid chromatography-tandem mass spectrometry data. Metabolomics, 2013, 9, 84-91.	1.4	35
65	MetFusion: integration of compound identification strategies. Journal of Mass Spectrometry, 2013, 48, 291-298.	0.7	163
66	MetaboLightsâ€"an open-access general-purpose repository for metabolomics studies and associated meta-data. Nucleic Acids Research, 2013, 41, D781-D786.	6.5	578
67	Tackling CASMI 2012: Solutions from MetFrag and MetFusion. Metabolites, 2013, 3, 623-636.	1.3	8
68	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. Metabolites, 2013, 3, 517-538.	1.3	35
69	CASMI: And the Winner is . . .. Metabolites, 2013, 3, 412-439.	1.3	30
70	Toward interoperable bioscience data. Nature Genetics, 2012, 44, 121-126.	9.4	362
71	TraMLâ€"A Standard Format for Exchange of Selected Reaction Monitoring Transition Lists. Molecular and Cellular Proteomics, 2012, 11, R111.015040.	2.5	65
72	CAMERA: An Integrated Strategy for Compound Spectra Extraction and Annotation of Liquid Chromatography/Mass Spectrometry Data Sets. Analytical Chemistry, 2012, 84, 283-289.	3.2	930

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73	A cross-platform toolkit for mass spectrometry and proteomics. Nature Biotechnology, 2012, 30, 918-920.	9.4	2,794
74	Consensus Structure Elucidation Combining GC/EI-MS, Structure Generation, and Calculated Properties. Analytical Chemistry, 2012, 84, 3287-3295.	3.2	57
75	Database supported candidate search for Metabolite identification. Journal of Integrative Bioinformatics, 2011, 8, 23-38.	1.0	9
76	mzMLâ€"a Community Standard for Mass Spectrometry Data. Molecular and Cellular Proteomics, 2011, 10, R110.000133.	2.5	555
77	Database supported candidate search for metabolite identification. Journal of Integrative Bioinformatics, 2011, 8, 157.	1.0	7
78	Meeting Report from the Second â€œMinimum Information for Biological and Biomedical Investigationsâ€• (MIBBI) workshop. Standards in Genomic Sciences, 2010, 3, 259-266.	1.5	32
79	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. Analytical and Bioanalytical Chemistry, 2010, 398, 2779-2788.	1.9	159
80	In silico fragmentation for computer assisted identification of metabolite mass spectra. BMC Bioinformatics, 2010, 11, 148.	1.2	541
81	MassBank: a public repository for sharing mass spectral data for life sciences. Journal of Mass Spectrometry, 2010, 45, 703-714.	0.7	1,831
82	ISA software suite: supporting standards-compliant experimental annotation and enabling curation at the community level. Bioinformatics, 2010, 26, 2354-2356.	1.8	247
83	Critical assessment of alignment procedures for LC-MS proteomics and metabolomics measurements. BMC Bioinformatics, 2008, 9, 375.	1.2	152
84	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. BMC Bioinformatics, 2008, 9, 400.	1.2	97
85	Highly sensitive feature detection for high resolution LC/MS. BMC Bioinformatics, 2008, 9, 504.	1.2	962
86	Metabolome Analysis of Biosynthetic Mutants Reveals a Diversity of Metabolic Changes and Allows Identification of a Large Number of New Compounds in Arabidopsis Â Â. Plant Physiology, 2008, 147, 2107-2120.	2.3	138
87	MetHouse: Raw and Preprocessed Mass Spectrometry Data. Journal of Integrative Bioinformatics, 2007, 4, 107-114.	1.0	5
88	Annotation of LC/ESI-MS Mass Signals. , 2007, , 371-380.		33
89	Fast Approximate Duplicate Detection for 2D-NMR Spectra. , 2007, , 139-155.		2
90	Database driven test case generation for protein-protein docking. Bioinformatics, 2005, 21, 683-684.	1.8	1

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91	Comparing bound and unbound protein structures using energy calculation and rotamer statistics. In Silico Biology, 2002, 2, 351-68.	0.4	3
92	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25
93	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3
94	Impact of in vitro hormone treatments on the bibenzyl production of Radula complanata. Botany, 0, , .	0.5	5