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	A cross-platform toolkit for mass spectrometry and proteomics. Nature Biotechnology, 2012, 30, 918-920.	9.4	2,794
2	MassBank: a public repository for sharing mass spectral data for life sciences. Journal of Mass Spectrometry, 2010, 45, 703-714.	0.7	1,831
3	Highly sensitive feature detection for high resolution LC/MS. BMC Bioinformatics, 2008, 9, 504.	1.2	962
4	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
5	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. Journal of Cheminformatics, 2016, 8, 3.	2.8	665
6	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	9.0	650
7	MetaboLightsâ€"an open-access general-purpose repository for metabolomics studies and associated meta-data. Nucleic Acids Research, 2013, 41, D781-D786.	6.5	578
8	mzMLâ€"a Community Standard for Mass Spectrometry Data. Molecular and Cellular Proteomics, 2011, 10, R110.000133.	2.5	555
9	In silico fragmentation for computer assisted identification of metabolite mass spectra. BMC Bioinformatics, 2010, 11, 148.	1.2	541
10	Mass appeal: metabolite identification in mass spectrometry-focused untargeted metabolomics. Metabolomics, 2013, 9, 44-66.	1.4	452
11	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
12	Mass spectrometry-based metabolomics: a guide for annotation, quantification and best reporting practices. Nature Methods, 2021, 18, 747-756.	9.0	403
13	Toward interoperable bioscience data. Nature Genetics, 2012, 44, 121-126.	9.4	362
14	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
15	IPO: a tool for automated optimization of XCMS parameters. BMC Bioinformatics, 2015, 16, 118.	1.2	249
16	ISA software suite: supporting standards-compliant experimental annotation and enabling curation at the community level. Bioinformatics, 2010, 26, 2354-2356.	1.8	247
17	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
18	RAMClust: A Novel Feature Clustering Method Enables Spectral-Matching-Based Annotation for Metabolomics Data. Analytical Chemistry, 2014, 86, 6812-6817.	3.2	219

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19	Metabolite identification: are you sure? And how do your peers gauge your confidence?. Metabolomics, 2014, 10, 350-353.	1.4	205
20	MetFusion: integration of compound identification strategies. Journal of Mass Spectrometry, 2013, 48, 291-298.	0.7	163
21	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
22	Computational mass spectrometry for metabolomics: Identification of metabolites and small molecules. Analytical and Bioanalytical Chemistry, 2010, 398, 2779-2788.	1.9	159
23	Critical assessment of alignment procedures for LC-MS proteomics and metabolomics measurements. BMC Bioinformatics, 2008, 9, 375.	1.2	152
24	Natural variation of root exudates in Arabidopsis thaliana-linking metabolomic and genomic data. Scientific Reports, 2016, 6, 29033.	1.6	143
25	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
26	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
27	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
28	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	2.8	122
29	PredRet: Prediction of Retention Time by Direct Mapping between Multiple Chromatographic Systems. Analytical Chemistry, 2015, 87, 9421-9428.	3.2	121
30	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	1.8	106
31	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. BMC Bioinformatics, 2008, 9, 400.	1.2	97
32	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
33	Discovering Regulated Metabolite Families in Untargeted Metabolomics Studies. Analytical Chemistry, 2016, 88, 8082-8090.	3.2	72
34	Comparative expression profiling reveals a role of the root apoplast in local phosphate response. BMC Plant Biology, 2016, 16, 106.	1.6	70
35	TraMLâ€"A Standard Format for Exchange of Selected Reaction Monitoring Transition Lists. Molecular and Cellular Proteomics, 2012, 11, R111.015040.	2.5	65
36	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64

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37	Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. Journal of Cheminformatics, 2021, 13, 19.	2.8	63
38	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
39	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
40	Consensus Structure Elucidation Combining GC/EI-MS, Structure Generation, and Calculated Properties. Analytical Chemistry, 2012, 84, 3287-3295.	3.2	57
41	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. Metabolites, 2018, 8, 51.	1.3	51
42	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
43	Bioinformatics can boost metabolomics research. Journal of Biotechnology, 2017, 261, 137-141.	1.9	49
44	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
45	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	1.8	47
46	Improving MetFrag with statistical learning of fragment annotations. BMC Bioinformatics, 2019, 20, 376.	1.2	44
47	mzTab-M: A Data Standard for Sharing Quantitative Results in Mass Spectrometry Metabolomics. Analytical Chemistry, 2019, 91, 3302-3310.	3.2	43
48	A Modular and Expandable Ecosystem for Metabolomics Data Annotation in R. Metabolites, 2022, 12, 173.	1.3	43
49	Functional Traits 2.0: The power of the metabolome for ecology. Journal of Ecology, 2022, 110, 4-20.	1.9	42
50	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
51	The significance of tree-tree interactions for forest ecosystem functioning. Basic and Applied Ecology, 2021, 55, 33-52.	1.2	38
52	Nearline acquisition and processing of liquid chromatography-tandem mass spectrometry data. Metabolomics, 2013, 9, 84-91.	1.4	35
53	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. Metabolites, 2013, 3, 517-538.	1.3	35
54	BiNChE: A web tool and library for chemical enrichment analysis based on the ChEBI ontology. BMC Bioinformatics, 2015, 16, 56.	1.2	35

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55	Networks and Graphs Discovery in Metabolomics Data Analysis and Interpretation. Frontiers in Molecular Biosciences, 2022, 9, 841373.	1.6	35
56	Chemical Diversity and Classification of Secondary Metabolites in Nine Bryophyte Species. Metabolites, 2019, 9, 222.	1.3	34
57	Seasonal variation of secondary metabolites in nine different bryophytes. Ecology and Evolution, 2018, 8, 9105-9117.	0.8	33
58	Annotation of LC/ESI-MS Mass Signals. , 2007, , 371-380.		33
59	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
60	CASMI: And the Winner is . . .. Metabolites, 2013, 3, 412-439.	1.3	30
61	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
62	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25
63	The Risa R/Bioconductor package: integrative data analysis from experimental metadata and back again. BMC Bioinformatics, 2014, 15, S11.	1.2	22
64	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
65	LipidFrag: Improving reliability of in silico fragmentation of lipids and application to the Caenorhabditis elegans lipidome. PLoS ONE, 2017, 12, e0172311.	1.1	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. Rapid Communications in Mass Spectrometry, 2015, 29, 1521-1529.	0.7	20
67	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
68	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
69	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
70	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
71	Prediction, Detection, and Validation of Isotope Clusters in Mass Spectrometry Data. Metabolites, 2016, 6, 37.	1.3	18
72	Computational annotation of plant metabolomics profiles via a novel network-assisted approach. Metabolomics, 2013, 9, 904-918.	1.4	17

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73	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. Mass Spectrometry, 2014, 3, S0036-S0036.	0.2	16
74	ChemFrag: Chemically meaningful annotation of fragment ion mass spectra. Journal of Mass Spectrometry, 2018, 53, 1104-1115.	0.7	14
75	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
76	Embedding standards in metabolomics: the Metabolomics Society data standards task group. Metabolomics, 2015, 11, 782-783.	1.4	13
77	Ontologies4Chem: the landscape of ontologies in chemistry. Pure and Applied Chemistry, 2022, 94, 605-622.	0.9	13
78	Computational workflow to study the seasonal variation of secondary metabolites in nine different bryophytes. Scientific Data, 2018, 5, 180179.	2.4	12
79	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
80	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
81	LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods. Scientific Data, 2021, 8, 52.	2.4	10
82	Modulation of Phosphate Deficiency-Induced Metabolic Changes by Iron Availability in Arabidopsis thaliana. International Journal of Molecular Sciences, 2021, 22, 7609.	1.8	10
83	Database supported candidate search for Metabolite identification. Journal of Integrative Bioinformatics, 2011, 8, 23-38.	1.0	9
84	Tackling CASMI 2012: Solutions from MetFrag and MetFusion. Metabolites, 2013, 3, 623-636.	1.3	8
85	Database supported candidate search for metabolite identification. Journal of Integrative Bioinformatics, 2011, 8, 157.	1.0	7
86	Metabolic drift in the aging nervous system is reflected in human cerebrospinal fluid. Scientific Reports, 2021, 11, 18822.	1.6	6
87	MetHouse: Raw and Preprocessed Mass Spectrometry Data. Journal of Integrative Bioinformatics, 2007, 4, 107-114.	1.0	5
88	Impact of in vitro hormone treatments on the bibenzyl production of Radula complanata. Botany, 0, , .	0.5	5
89	Data format standards in analytical chemistry. Pure and Applied Chemistry, 2022, 94, 725-736.	0.9	4
90	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3

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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	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
93	Fast Approximate Duplicate Detection for 2D-NMR Spectra. , 2007, , 139-155.		2
94	Database driven test case generation for protein-protein docking. Bioinformatics, 2005, 21, 683-684.	1.8	1