Kai DÃ¼hrkop

List of Publications by Year
in descending order

27 papers	3,832 citations	430874 18 h-index	526287 27 g-index
37 all docs	37 docs citations	37 times ranked	3494 citing authors

#	Article	IF	Citations
1	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nature Methods, 2019, 16, 299-302.	19.0	822
2	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12580-12585.	7.1	695
3	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
4	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. Nature Biotechnology, 2021, 39, 462-471.	17.5	317
5	Fragmentation trees reloaded. Journal of Cheminformatics, 2016, 8, 5.	6.1	138
6	Significance estimation for large scale metabolomics annotations by spectral matching. Nature Communications, 2017, 8, 1494.	12.8	128
7	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	6.1	122
8	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. Nature Communications, 2021, 12, 3832.	12.8	119
9	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	4.1	106
10	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. Nature Machine Intelligence, 2020, 2, 629-641.	16.0	103
11	High-confidence structural annotation of metabolites absent from spectral libraries. Nature Biotechnology, 2022, 40, 411-421.	17.5	100
12	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	4.1	87
13	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. Nature Chemical Biology, 2021, 17, 146-151.	8.0	73
14	Fast metabolite identification with Input Output Kernel Regression. Bioinformatics, 2016, 32, i28-i36.	4.1	57
15	MSNovelist: de novo structure generation from mass spectra. Nature Methods, 2022, 19, 865-870.	19.0	49
16	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. Bioinformatics, 2018, 34, i333-i340.	4.1	36
17	Molecular Formula Identification with SIRIUS. Metabolites, 2013, 3, 506-516.	2.9	34
18	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.6	20

#	Article	IF	Citations
19	Fast alignment of fragmentation trees. Bioinformatics, 2012, 28, i265-i273.	4.1	14
20	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. Methods in Molecular Biology, 2020, 2104, 185-207.	0.9	11
21	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.3	6
22	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.3	6
23	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.3	5
24	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. Environmental Science & Technology, 2022, 56, 11027-11040.	10.0	5
25	Studying Charge Migration Fragmentation of Sodiated Precursor Ions in Collision-Induced Dissociation at the Library Scale. Journal of the American Society for Mass Spectrometry, 2021, 32, 180-186.	2.8	4
26	Deep kernel learning improves molecular fingerprint prediction from tandem mass spectra. Bioinformatics, 2022, 38, i342-i349.	4.1	4
27	Computational methods for small molecule identification. IT - Information Technology, 2019, 61, 285-292.	0.9	0