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	High-confidence structural annotation of metabolites absent from spectral libraries. Nature Biotechnology, 2022, 40, 411-421.	17.5	100
2	Deep kernel learning improves molecular fingerprint prediction from tandem mass spectra. Bioinformatics, 2022, 38, i342-i349.	4.1	4
3	MSNovelist: de novo structure generation from mass spectra. Nature Methods, 2022, 19, 865-870.	19.0	49
4	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. Environmental Science & Technology, 2022, 56, 11027-11040.	10.0	5
5	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. Nature Biotechnology, 2021, 39, 462-471.	17.5	317
6	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
7	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. Nature Chemical Biology, 2021, 17, 146-151.	8.0	73
8	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. Nature Communications, 2021, 12, 3832.	12.8	119
9	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. Nature Machine Intelligence, 2020, 2, 629-641.	16.0	103
10	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
11	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. Methods in Molecular Biology, 2020, 2104, 185-207.	0.9	11
12	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nature Methods, 2019, 16, 299-302.	19.0	822
13	Computational methods for small molecule identification. IT - Information Technology, 2019, 61, 285-292.	0.9	0
14	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. Bioinformatics, 2018, 34, i333-i340.	4.1	36
15	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	4.1	106
16	Significance estimation for large scale metabolomics annotations by spectral matching. Nature Communications, 2017, 8, 1494.	12.8	128
17	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	6.1	122
18	Fast metabolite identification with Input Output Kernel Regression. Bioinformatics, 2016, 32, i28-i36.	4.1	57

#	Article	IF	Citations
19	Fragmentation trees reloaded. Journal of Cheminformatics, 2016, 8, 5.	6.1	138
20	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
21	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.3	6
22	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.3	5
23	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.6	20
24	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	4.1	87
25	Molecular Formula Identification with SIRIUS. Metabolites, 2013, 3, 506-516.	2.9	34
26	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.3	6
27	Fast alignment of fragmentation trees. Bioinformatics, 2012, 28, i265-i273.	4.1	14