

# Kai DÃ¼hrkop

## List of Publications by Year in descending order

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Version: 2024-02-01

27  
papers

3,832  
citations

430442

18  
h-index

525886

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. <i>Nature Biotechnology</i> , 2022, 40, 411-421.	9.4	100
2	Deep kernel learning improves molecular fingerprint prediction from tandem mass spectra. <i>Bioinformatics</i> , 2022, 38, i342-i349.	1.8	4
3	MSNovelist: de novo structure generation from mass spectra. <i>Nature Methods</i> , 2022, 19, 865-870.	9.0	49
4	Mass Difference Matching Unfolds Hidden Molecular Structures of Dissolved Organic Matter. <i>Environmental Science &amp; Technology</i> , 2022, 56, 11027-11040.	4.6	5
5	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. <i>Nature Biotechnology</i> , 2021, 39, 462-471.	9.4	317
6	Studying Charge Migration Fragmentation of Sodiated Precursor Ions in Collision-Induced Dissociation at the Library Scale. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 180-186.	1.2	4
7	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. <i>Nature Chemical Biology</i> , 2021, 17, 146-151.	3.9	73
8	Ion identity molecular networking for mass spectrometry-based metabolomics in the GNPS environment. <i>Nature Communications</i> , 2021, 12, 3832.	5.8	119
9	Database-independent molecular formula annotation using Gibbs sampling through ZODIAC. <i>Nature Machine Intelligence</i> , 2020, 2, 629-641.	8.3	103
10	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , 2020, 17, 905-908.	9.0	650
11	De Novo Molecular Formula Annotation and Structure Elucidation Using SIRIUS 4. <i>Methods in Molecular Biology</i> , 2020, 2104, 185-207.	0.4	11
12	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. <i>Nature Methods</i> , 2019, 16, 299-302.	9.0	822
13	Computational methods for small molecule identification. <i>IT - Information Technology</i> , 2019, 61, 285-292.	0.6	0
14	Bayesian networks for mass spectrometric metabolite identification via molecular fingerprints. <i>Bioinformatics</i> , 2018, 34, i333-i340.	1.8	36
15	Current Challenges in Plant Eco-Metabolomics. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1385.	1.8	106
16	Significance estimation for large scale metabolomics annotations by spectral matching. <i>Nature Communications</i> , 2017, 8, 1494.	5.8	128
17	Critical Assessment of Small Molecule Identification 2016: automated methods. <i>Journal of Cheminformatics</i> , 2017, 9, 22.	2.8	122
18	Fast metabolite identification with Input Output Kernel Regression. <i>Bioinformatics</i> , 2016, 32, i28-i36.	1.8	57

#	ARTICLE	IF	CITATIONS
19	Fragmentation trees reloaded. Journal of Cheminformatics, 2016, 8, 5.	2.8	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.	3.3	695
21	Fragmentation Trees Reloaded. Lecture Notes in Computer Science, 2015, , 65-79.	1.0	6
22	Speedy Colorful Subtrees. Lecture Notes in Computer Science, 2015, , 310-322.	1.0	5
23	Molecular Formula Identification Using Isotope Pattern Analysis and Calculation of Fragmentation Trees. Mass Spectrometry, 2014, 3, S0037-S0037.	0.2	20
24	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	1.8	87
25	Molecular Formula Identification with SIRIUS. Metabolites, 2013, 3, 506-516.	1.3	34
26	Faster Mass Decomposition. Lecture Notes in Computer Science, 2013, , 45-58.	1.0	6
27	Fast alignment of fragmentation trees. Bioinformatics, 2012, 28, i265-i273.	1.8	14