Tobias Kind

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

75 papers	8,735 citations	38 h-index	85 g-index
85 ext. papers	10,764 ext. citations	7.5 avg, IF	6.21 L-index

#	Paper	IF	Citations
75	MS-DIAL: data-independent MS/MS deconvolution for comprehensive metabolome analysis. *Nature Methods*, **2015**, 12, 523-6	21.6	1036
74	FiehnLib: mass spectral and retention index libraries for metabolomics based on quadrupole and time-of-flight gas chromatography/mass spectrometry. *Analytical Chemistry*, **2009**, 81, 10038-48	7.8	939
73	Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry. *BMC Bioinformatics*, **2007**, 8, 105	3.6	777
72	LipidBlast in silico tandem mass spectrometry database for lipid identification. *Nature Methods*, **2013**, 10, 755-8	21.6	550
71	Metabolomic database annotations via query of elemental compositions: mass accuracy is insufficient even at less than 1 ppm. *BMC Bioinformatics*, **2006**, 7, 234	3.6	470
70	Quality control for plant metabolomics: reporting MSI-compliant studies. *Plant Journal*, **2008**, 53, 691-704	4.9	457
69	A comprehensive urinary metabolomic approach for identifying kidney cancerr. *Analytical Biochemistry*, **2007**, 363, 185-95	3.1	405
68	Advances in structure elucidation of small molecules using mass spectrometry. *Bioanalytical Reviews*, **2010**, 2, 23-60	1	343
67	Mass spectrometry-based metabolic profiling reveals different metabolite patterns in invasive ovarian carcinomas and ovarian borderline tumors. *Cancer Research*, **2006**, 66, 10795-804	10.1	323
66	Hydrogen Rearrangement Rules: Computational MS/MS Fragmentation and Structure Elucidation Using MS-FINDER Software. *Analytical Chemistry*, **2016**, 88, 7946-58	7.8	292
65	Software Tools and Approaches for Compound Identification of LC-MS/MS Data in Metabolomics. *Metabolites*, **2018**, 8,	5.6	253
64	Metabolite profiling of human colon carcinoma--deregulation of TCA cycle and amino acid turnover. *Molecular Cancer*, **2008**, 7, 72	42.1	235
63	Identifying metabolites by integrating metabolome databases with mass spectrometry cheminformatics. *Nature Methods*, **2018**, 15, 53-56	21.6	200
62	Identification of small molecules using accurate mass MS/MS search. *Mass Spectrometry Reviews*, **2018**, 37, 513-532	11	194
61	MetaMapp: mapping and visualizing metabolomic data by integrating information from biochemical pathways and chemical and mass spectral similarity. *BMC Bioinformatics*, **2012**, 13, 99	3.6	161
60	MINEs: open access databases of computationally predicted enzyme promiscuity products for untargeted metabolomics. *Journal of Cheminformatics*, **2015**, 7, 44	8.6	137
59	How large is the metabolome? A critical analysis of data exchange practices in chemistry. *PLoS ONE*, **2009**, 4, e5440	3.7	94

58	Critical Assessment of Small Molecule Identification 2016: automated methods. *Journal of Cheminformatics*, **2017**, 9, 22	8.6	89
57	The Chemical Translation Service--a web-based tool to improve standardization of metabolomic reports. *Bioinformatics*, **2010**, 26, 2647-8	7.2	86
56	Systematic Error Removal Using Random Forest for Normalizing Large-Scale Untargeted Lipidomics Data. *Analytical Chemistry*, **2019**, 91, 3590-3596	7.8	82
55	Metabolite profiling in blood plasma. *Methods in Molecular Biology*, **2007**, 358, 3-17	1.4	81
54	Extending biochemical databases by metabolomic surveys.. *Journal of Biological Chemistry*, **2011**, 286, 30244	5.4	78
53	Structure Annotation of All Mass Spectra in Untargeted Metabolomics. *Analytical Chemistry*, **2019**, 91, 2155-2162	7.8	78
52	MS2Analyzer: A software for small molecule substructure annotations from accurate tandem mass spectra. *Analytical Chemistry*, **2014**, 86, 10724-31	7.8	67
51	Applying in-silico retention index and mass spectra matching for identification of unknown metabolites in accurate mass GC-TOF mass spectrometry. *Analytical Chemistry*, **2011**, 83, 5895-902	7.8	67
50	Comprehensive comparison of in silico MS/MS fragmentation tools of the CASMI contest: database boosting is needed to achieve 93% accuracy. *Journal of Cheminformatics*, **2017**, 9, 32	8.6	64
49	Extending biochemical databases by metabolomic surveys. *Journal of Biological Chemistry*, **2011**, 286, 23637-43	5.4	61
48	Effect-directed fractionation and identification of cytochrome P4501A-inducing halogenated aromatic hydrocarbons in a contaminated sediment. *Environmental Toxicology and Chemistry*, **2002**, 21, 2654-2662	3.8	59
47	Qualitative analysis of algal secretions with multiple mass spectrometric platforms. *Journal of Chromatography A*, **2012**, 1244, 139-47	4.5	56
46	Induced pluripotent stem cells show metabolomic differences to embryonic stem cells in polyunsaturated phosphatidylcholines and primary metabolism. *PLoS ONE*, **2012**, 7, e46770	3.7	54
45	An in silico MS/MS library for automatic annotation of novel FAHFA lipids. *Journal of Cheminformatics*, **2015**, 7, 53	8.6	51
44	Identification of naturally occurring fatty acids of the myelin sheath that resolve neuroinflammation. *Science Translational Medicine*, **2012**, 4, 137ra73	17.5	51
43	Increasing Compound Identification Rates in Untargeted Lipidomics Research with Liquid Chromatography Drift Time-Ion Mobility Mass Spectrometry. *Analytical Chemistry*, **2018**, 90, 10758-10764	7.8	49
42	Determination of elemental compositions by gas chromatography/time-of-flight mass spectrometry using chemical and electron ionization. *Rapid Communications in Mass Spectrometry*, **2010**, 24, 1172-80	2.2	48
41	Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. *Environmental Pollution*, **2003**, 121, 81-5	9.3	47

40	Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. *Analytical Chemistry*, **2020**, 92, 7515-7522	7.8	44
39	Cofactor symbiosis for enhanced algal growth, biofuel production, and wastewater treatment. *Algal Research*, **2016**, 17, 308-315	5	43
38	Sequential fractionation procedure for the identification of potentially cytochrome P4501A-inducing compounds. *Journal of Chromatography A*, **2003**, 986, 55-66	4.5	39
37	LipidBlast templates as flexible tools for creating new in-silico tandem mass spectral libraries. *Analytical Chemistry*, **2014**, 86, 11024-7	7.8	38
36	Pharmacogenetics meets metabolomics: discovery of tryptophan as a new endogenous OCT2 substrate related to metformin disposition. *PLoS ONE*, **2012**, 7, e36637	3.7	38
35	Retention projection enables accurate calculation of liquid chromatographic retention times across labs and methods. *Journal of Chromatography A*, **2015**, 1412, 43-51	4.5	37
34	Comparative evaluation of extraction methods for simultaneous mass-spectrometric analysis of complex lipids and primary metabolites from human blood plasma. *Analytical and Bioanalytical Chemistry*, **2014**, 406, 7275-86	4.4	37
33	Lipidomic Analysis of Chlamydomonas reinhardtii under Nitrogen and Sulfur Deprivation. *PLoS ONE*, **2015**, 10, e0137948	3.7	35
32	Use of boiling point□ee retention index correlation for rapid review of gas chromatography-mass spectrometry data. *Analytica Chimica Acta*, **2003**, 494, 235-243	6.6	30
31	Prognostic impact of AMP-activated protein kinase expression in ovarian carcinoma: correlation of protein expression and GC/TOF-MS-based metabolomics. *Oncology Reports*, **2011**, 25, 1005-12	3.5	27
30	Interstitial Cystitis-Associated Urinary Metabolites Identified by Mass-Spectrometry Based Metabolomics Analysis. *Scientific Reports*, **2016**, 6, 39227	4.9	27
29	Hydrocarbon phenotyping of algal species using pyrolysis-gas chromatography mass spectrometry. *BMC Biotechnology*, **2010**, 10, 40	3.5	24
28	Changes in plasma metabolites and glucose homeostasis during omega-3 polyunsaturated fatty acid supplementation in women with polycystic ovary syndrome. *BBA Clinical*, **2016**, 5, 179-85		24
27	Role of squalene in the organization of monolayers derived from lipid extracts of Halobacterium salinarum. *Langmuir*, **2013**, 29, 7922-30	4	23
26	Ultrafast Polyphenol Metabolomics of Red Wines Using MicroLC-MS/MS. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 505-12	5.7	22
25	Using Accurate Mass Gas Chromatography-Mass Spectrometry with the MINE Database for Epimetabolite Annotation. *Analytical Chemistry*, **2017**, 89, 10171-10180	7.8	20
24	A Comprehensive Plasma Metabolomics Dataset for a Cohort of Mouse Knockouts within the International Mouse Phenotyping Consortium. *Metabolites*, **2019**, 9,	5.6	19
23	Quantum Chemistry Calculations for Metabolomics. *Chemical Reviews*, **2021**, 121, 5633-5670	68.1	18

22	Strategies for dereplication of natural compounds using high-resolution tandem mass spectrometry. *Phytochemistry Letters*, **2017**, 21, 313-319	1.9	17
21	Informatics for improved algal taxonomic classification and research: A case study of UTEX 2341. *Algal Research*, **2015**, 12, 545-549	5	15
20	Longitudinal Metabolome-Wide Signals Prior to the Appearance of a First Islet Autoantibody in Children Participating in the TEDDY Study. *Diabetes*, **2020**, 69, 465-476	0.9	13
19	Predicting in silico electron ionization mass spectra using quantum chemistry. *Journal of Cheminformatics*, **2020**, 12, 63	8.6	12
18	Environmental Tobacco Smoke Alters Metabolic Systems in Adult Rats. *Chemical Research in Toxicology*, **2016**, 29, 1818-1827	4	12
17	Data Processing, Metabolomic Databases and Pathway Analysis **2011**, 367-406		11
16	In-Silico-Generated Library for Sensitive Detection of 2-Dimethylaminoethylamine Derivatized FAHFA Lipids Using High-Resolution Tandem Mass Spectrometry. *Analytical Chemistry*, **2020**, 92, 5960-5968	7.8	9
15	Effect of steroidal saponins from Agave on the polysaccharide cell wall composition of Saccharomyces cerevisiae and Kluyveromyces marxianus. *LWT - Food Science and Technology*, **2017**, 77, 430-439	5.4	9
14	Exploration of polar lipid accumulation profiles in Euglena gracilis using LipidBlast, an MS/MS spectral library constructed in silico. *Bioscience, Biotechnology and Biochemistry*, **2014**, 78, 14-8	2.1	9
13	A Large and Phylogenetically Diverse Class of Type 1 Opsins Lacking a Canonical Retinal Binding Site. *PLoS ONE*, **2016**, 11, e0156543	3.7	7
12	Spectral entropy outperforms MS/MS dot product similarity for small-molecule compound identification. *Nature Methods*, **2021**, 18, 1524-1531	21.6	7
11	Hyperosmotic stress in Chlamydomonas induces metabolomic changes in biosynthesis of complex lipids. *European Journal of Phycology*, **2020**, 55, 11-29	2.2	7
10	Age and sex are associated with the plasma lipidome: findings from the GOLDN study. *Lipids in Health and Disease*, **2021**, 20, 30	4.4	6
9	Software platform virtualization in chemistry research and university teaching. *Journal of Cheminformatics*, **2009**, 1, 18	8.6	4
8	A lipidome-wide association study of the lipoprotein insulin resistance index. *Lipids in Health and Disease*, **2020**, 19, 153	4.4	2
7	Analysis of Polar Lipids inChlamydomonas reinhardtiiUsing Nanoelectrospray Direct Infusion Method and Gas Chromatography and Mass Spectrometric Detection. *Acta Chimica Sinica*, **2013**, 71, 663	3.3	2
6	Advances in structure elucidation of small molecules using mass spectrometry **2013**, 129-166		2
5	Metabolomics Analyses of 14 Classical Neurotransmitters by GC-TOF with LC-MS Illustrates Secretion of 9 Cell-Cell Signaling Molecules from Sympathoadrenal Chromaffin Cells in the Presence of Lithium. *ACS Chemical Neuroscience*, **2019**, 10, 1369-1379	5.7	1

4	Data Processing, Metabolomic Databases and Pathway Analysis **2018**, 367-406		1
3	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites.. *Analytical Chemistry*, **2022**,	7.8	1
2	Changes in lipidomic profile by anti-retroviral treatment regimen: An ACTG 5257 ancillary study. *Medicine (United States)*, **2021**, 100, e26588	1.8	0
1	An Amish founder population reveals rare-population genetic determinants of the human lipidome.. *Communications Biology*, **2022**, 5, 334	6.7	0