

Tobias Kind

List of Publications by Year in Descending Order

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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	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites.. <i>Analytical Chemistry</i> , 2022 ,	7.8	1
74	An Amish founder population reveals rare-population genetic determinants of the human lipidome.. <i>Communications Biology</i> , 2022 , 5, 334	6.7	0
73	Spectral entropy outperforms MS/MS dot product similarity for small-molecule compound identification. <i>Nature Methods</i> , 2021 , 18, 1524-1531	21.6	7
72	Age and sex are associated with the plasma lipidome: findings from the GOLDN study. <i>Lipids in Health and Disease</i> , 2021 , 20, 30	4.4	6
71	Quantum Chemistry Calculations for Metabolomics. <i>Chemical Reviews</i> , 2021 , 121, 5633-5670	68.1	18
70	Changes in lipidomic profile by anti-retroviral treatment regimen: An ACTG 5257 ancillary study. <i>Medicine (United States)</i> , 2021 , 100, e26588	1.8	0
69	Predicting in silico electron ionization mass spectra using quantum chemistry. <i>Journal of Cheminformatics</i> , 2020 , 12, 63	8.6	12
68	Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. <i>Analytical Chemistry</i> , 2020 , 92, 7515-7522	7.8	44
67	Longitudinal Metabolome-Wide Signals Prior to the Appearance of a First Islet Autoantibody in Children Participating in the TEDDY Study. <i>Diabetes</i> , 2020 , 69, 465-476	0.9	13
66	In-Silico-Generated Library for Sensitive Detection of 2-Dimethylaminoethylamine Derivatized FAHFA Lipids Using High-Resolution Tandem Mass Spectrometry. <i>Analytical Chemistry</i> , 2020 , 92, 5960-5968	7.8	9
65	A lipidome-wide association study of the lipoprotein insulin resistance index. <i>Lipids in Health and Disease</i> , 2020 , 19, 153	4.4	2
64	Hyperosmotic stress in Chlamydomonas induces metabolomic changes in biosynthesis of complex lipids. <i>European Journal of Phycology</i> , 2020 , 55, 11-29	2.2	7
63	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. <i>ACS Chemical Neuroscience</i> , 2019 , 10, 1369-1379	5.7	1
62	A Comprehensive Plasma Metabolomics Dataset for a Cohort of Mouse Knockouts within the International Mouse Phenotyping Consortium. <i>Metabolites</i> , 2019 , 9,	5.6	19
61	Systematic Error Removal Using Random Forest for Normalizing Large-Scale Untargeted Lipidomics Data. <i>Analytical Chemistry</i> , 2019 , 91, 3590-3596	7.8	82
60	Structure Annotation of All Mass Spectra in Untargeted Metabolomics. <i>Analytical Chemistry</i> , 2019 , 91, 2155-2162	7.8	78
59	Identification of small molecules using accurate mass MS/MS search. <i>Mass Spectrometry Reviews</i> , 2018 , 37, 513-532	11	194

58	Software Tools and Approaches for Compound Identification of LC-MS/MS Data in Metabolomics. <i>Metabolites</i> , 2018 , 8,	5.6	253
57	Increasing Compound Identification Rates in Untargeted Lipidomics Research with Liquid Chromatography Drift Time-Ion Mobility Mass Spectrometry. <i>Analytical Chemistry</i> , 2018 , 90, 10758-10764	7.8	49
56	Data Processing, Metabolomic Databases and Pathway Analysis 2018 , 367-406		1
55	Identifying metabolites by integrating metabolome databases with mass spectrometry cheminformatics. <i>Nature Methods</i> , 2018 , 15, 53-56	21.6	200
54	Using Accurate Mass Gas Chromatography-Mass Spectrometry with the MINE Database for Epimetabolite Annotation. <i>Analytical Chemistry</i> , 2017 , 89, 10171-10180	7.8	20
53	Critical Assessment of Small Molecule Identification 2016: automated methods. <i>Journal of Cheminformatics</i> , 2017 , 9, 22	8.6	89
52	Comprehensive comparison of in silico MS/MS fragmentation tools of the CASMI contest: database boosting is needed to achieve 93% accuracy. <i>Journal of Cheminformatics</i> , 2017 , 9, 32	8.6	64
51	Strategies for dereplication of natural compounds using high-resolution tandem mass spectrometry. <i>Phytochemistry Letters</i> , 2017 , 21, 313-319	1.9	17
50	Effect of steroidal saponins from Agave on the polysaccharide cell wall composition of <i>Saccharomyces cerevisiae</i> and <i>Kluyveromyces marxianus</i> . <i>LWT - Food Science and Technology</i> , 2017 , 77, 430-439	5.4	9
49	Hydrogen Rearrangement Rules: Computational MS/MS Fragmentation and Structure Elucidation Using MS-FINDER Software. <i>Analytical Chemistry</i> , 2016 , 88, 7946-58	7.8	292
48	Environmental Tobacco Smoke Alters Metabolic Systems in Adult Rats. <i>Chemical Research in Toxicology</i> , 2016 , 29, 1818-1827	4	12
47	Cofactor symbiosis for enhanced algal growth, biofuel production, and wastewater treatment. <i>Algal Research</i> , 2016 , 17, 308-315	5	43
46	Ultrafast Polyphenol Metabolomics of Red Wines Using MicroLC-MS/MS. <i>Journal of Agricultural and Food Chemistry</i> , 2016 , 64, 505-12	5.7	22
45	A Large and Phylogenetically Diverse Class of Type 1 Opsins Lacking a Canonical Retinal Binding Site. <i>PLoS ONE</i> , 2016 , 11, e0156543	3.7	7
44	Interstitial Cystitis-Associated Urinary Metabolites Identified by Mass-Spectrometry Based Metabolomics Analysis. <i>Scientific Reports</i> , 2016 , 6, 39227	4.9	27
43	Changes in plasma metabolites and glucose homeostasis during omega-3 polyunsaturated fatty acid supplementation in women with polycystic ovary syndrome. <i>BBA Clinical</i> , 2016 , 5, 179-85		24
42	Retention projection enables accurate calculation of liquid chromatographic retention times across labs and methods. <i>Journal of Chromatography A</i> , 2015 , 1412, 43-51	4.5	37
41	MS-DIAL: data-independent MS/MS deconvolution for comprehensive metabolome analysis. <i>Nature Methods</i> , 2015 , 12, 523-6	21.6	1036

40	MINEs: open access databases of computationally predicted enzyme promiscuity products for untargeted metabolomics. <i>Journal of Cheminformatics</i> , 2015 , 7, 44	8.6	137
39	Informatics for improved algal taxonomic classification and research: A case study of UTEX 2341. <i>Algal Research</i> , 2015 , 12, 545-549	5	15
38	An in silico MS/MS library for automatic annotation of novel FAHFA lipids. <i>Journal of Cheminformatics</i> , 2015 , 7, 53	8.6	51
37	Lipidomic Analysis of <i>Chlamydomonas reinhardtii</i> under Nitrogen and Sulfur Deprivation. <i>PLoS ONE</i> , 2015 , 10, e0137948	3.7	35
36	LipidBlast templates as flexible tools for creating new in-silico tandem mass spectral libraries. <i>Analytical Chemistry</i> , 2014 , 86, 11024-7	7.8	38
35	MS2Analyzer: A software for small molecule substructure annotations from accurate tandem mass spectra. <i>Analytical Chemistry</i> , 2014 , 86, 10724-31	7.8	67
34	Exploration of polar lipid accumulation profiles in <i>Euglena gracilis</i> using LipidBlast, an MS/MS spectral library constructed in silico. <i>Bioscience, Biotechnology and Biochemistry</i> , 2014 , 78, 14-8	2.1	9
33	Comparative evaluation of extraction methods for simultaneous mass-spectrometric analysis of complex lipids and primary metabolites from human blood plasma. <i>Analytical and Bioanalytical Chemistry</i> , 2014 , 406, 7275-86	4.4	37
32	LipidBlast in silico tandem mass spectrometry database for lipid identification. <i>Nature Methods</i> , 2013 , 10, 755-8	21.6	550
31	Role of squalene in the organization of monolayers derived from lipid extracts of <i>Halobacterium salinarum</i> . <i>Langmuir</i> , 2013 , 29, 7922-30	4	23
30	Analysis of Polar Lipids in <i>Chlamydomonas reinhardtii</i> Using Nanoelectrospray Direct Infusion Method and Gas Chromatography and Mass Spectrometric Detection. <i>Acta Chimica Sinica</i> , 2013 , 71, 663	3.3	2
29	Advances in structure elucidation of small molecules using mass spectrometry 2013 , 129-166		2
28	MetaMapp: mapping and visualizing metabolomic data by integrating information from biochemical pathways and chemical and mass spectral similarity. <i>BMC Bioinformatics</i> , 2012 , 13, 99	3.6	161
27	Pharmacogenetics meets metabolomics: discovery of tryptophan as a new endogenous OCT2 substrate related to metformin disposition. <i>PLoS ONE</i> , 2012 , 7, e36637	3.7	38
26	Qualitative analysis of algal secretions with multiple mass spectrometric platforms. <i>Journal of Chromatography A</i> , 2012 , 1244, 139-47	4.5	56
25	Induced pluripotent stem cells show metabolomic differences to embryonic stem cells in polyunsaturated phosphatidylcholines and primary metabolism. <i>PLoS ONE</i> , 2012 , 7, e46770	3.7	54
24	Identification of naturally occurring fatty acids of the myelin sheath that resolve neuroinflammation. <i>Science Translational Medicine</i> , 2012 , 4, 137ra73	17.5	51
23	Applying in-silico retention index and mass spectra matching for identification of unknown metabolites in accurate mass GC-TOF mass spectrometry. <i>Analytical Chemistry</i> , 2011 , 83, 5895-902	7.8	67

22	Prognostic impact of AMP-activated protein kinase expression in ovarian carcinoma: correlation of protein expression and GC/TOF-MS-based metabolomics. <i>Oncology Reports</i> , 2011 , 25, 1005-12	3.5	27
21	Data Processing, Metabolomic Databases and Pathway Analysis 2011 , 367-406		11
20	Extending biochemical databases by metabolomic surveys.. <i>Journal of Biological Chemistry</i> , 2011 , 286, 30244	5.4	78
19	Extending biochemical databases by metabolomic surveys. <i>Journal of Biological Chemistry</i> , 2011 , 286, 23637-43	5.4	61
18	The Chemical Translation Service--a web-based tool to improve standardization of metabolomic reports. <i>Bioinformatics</i> , 2010 , 26, 2647-8	7.2	86
17	Advances in structure elucidation of small molecules using mass spectrometry. <i>Bioanalytical Reviews</i> , 2010 , 2, 23-60	1	343
16	Hydrocarbon phenotyping of algal species using pyrolysis-gas chromatography mass spectrometry. <i>BMC Biotechnology</i> , 2010 , 10, 40	3.5	24
15	Determination of elemental compositions by gas chromatography/time-of-flight mass spectrometry using chemical and electron ionization. <i>Rapid Communications in Mass Spectrometry</i> , 2010 , 24, 1172-80	2.2	48
14	Software platform virtualization in chemistry research and university teaching. <i>Journal of Cheminformatics</i> , 2009 , 1, 18	8.6	4
13	FiehnLib: mass spectral and retention index libraries for metabolomics based on quadrupole and time-of-flight gas chromatography/mass spectrometry. <i>Analytical Chemistry</i> , 2009 , 81, 10038-48	7.8	939
12	How large is the metabolome? A critical analysis of data exchange practices in chemistry. <i>PLoS ONE</i> , 2009 , 4, e5440	3.7	94
11	Quality control for plant metabolomics: reporting MSI-compliant studies. <i>Plant Journal</i> , 2008 , 53, 691-704	4.9	457
10	Metabolite profiling of human colon carcinoma--deregulation of TCA cycle and amino acid turnover. <i>Molecular Cancer</i> , 2008 , 7, 72	42.1	235
9	A comprehensive urinary metabolomic approach for identifying kidney cancer. <i>Analytical Biochemistry</i> , 2007 , 363, 185-95	3.1	405
8	Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry. <i>BMC Bioinformatics</i> , 2007 , 8, 105	3.6	777
7	Metabolite profiling in blood plasma. <i>Methods in Molecular Biology</i> , 2007 , 358, 3-17	1.4	81
6	Metabolomic database annotations via query of elemental compositions: mass accuracy is insufficient even at less than 1 ppm. <i>BMC Bioinformatics</i> , 2006 , 7, 234	3.6	470
5	Mass spectrometry-based metabolic profiling reveals different metabolite patterns in invasive ovarian carcinomas and ovarian borderline tumors. <i>Cancer Research</i> , 2006 , 66, 10795-804	10.1	323

4	Use of boiling point/retention index correlation for rapid review of gas chromatography-mass spectrometry data. <i>Analytica Chimica Acta</i> , 2003 , 494, 235-243	6.6	30
3	Sequential fractionation procedure for the identification of potentially cytochrome P4501A-inducing compounds. <i>Journal of Chromatography A</i> , 2003 , 986, 55-66	4.5	39
2	Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. <i>Environmental Pollution</i> , 2003 , 121, 81-5	9.3	47
1	Effect-directed fractionation and identification of cytochrome P4501A-inducing halogenated aromatic hydrocarbons in a contaminated sediment. <i>Environmental Toxicology and Chemistry</i> , 2002 , 21, 2654-2662	3.8	59