Tobias Kind

List of Publications by Year
in descending order

78 papers	12,200 citations	66343 42 h-index	74163 75 g-index
85 all docs	85 docs citations	85 times ranked	14330 citing authors

#	Article	IF	Citations
1	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites. Analytical Chemistry, 2022, , .	6.5	5
2	Evaluating the Accuracy of the QCEIMS Approach for Computational Prediction of Electron Ionization Mass Spectra of Purines and Pyrimidines. Metabolites, 2022, 12, 68.	2.9	4
3	Acyl-CoA Identification in Mouse Liver Samples Using the In Silico CoA-Blast Tandem Mass Spectral Library. Analytical Chemistry, 2022, 94, 2732-2739.	6.5	6
4	An Amish founder population reveals rare-population genetic determinants of the human lipidome. Communications Biology, 2022, 5, 334.	4.4	7
5	Age and sex are associated with the plasma lipidome: findings from the GOLDN study. Lipids in Health and Disease, 2021, 20, 30.	3.0	36
6	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	47.7	47
7	Changes in lipidomic profile by anti-retroviral treatment regimen. Medicine (United States), 2021, 100, e26588.	1.0	1
8	Genomics of Postprandial Lipidomics in the Genetics of Lipid-Lowering Drugs and Diet Network Study. Nutrients, 2021, 13, 4000.	4.1	2
9	Spectral entropy outperforms MS/MS dot product similarity for small-molecule compound identification. Nature Methods, 2021, 18, 1524-1531.	19.0	71
10	Hyperosmotic stress in Chlamydomonas induces metabolomic changes in biosynthesis of complex lipids. European Journal of Phycology, 2020, 55, 11-29.	2.0	11
11	Predicting in silico electron ionization mass spectra using quantum chemistry. Journal of Cheminformatics, 2020, 12, 63.	6.1	20
12	Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. Analytical Chemistry, 2020, 92, 7515-7522.	6.5	128
13	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.	0.6	30
14	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.	6.5	23
15	A lipidome-wide association study of the lipoprotein insulin resistance index. Lipids in Health and Disease, 2020, 19, 153.	3.0	6
16	Metabolomics Analyses of 14 Classical Neurotransmitters by GC-TOF with LC-MS Illustrates Secretion of 9 Cellâ€“Cell Signaling Molecules from Sympathoadrenal Chromaffin Cells in the Presence of Lithium. ACS Chemical Neuroscience, 2019, 10, 1369-1379.	3.5	13
17	A Comprehensive Plasma Metabolomics Dataset for a Cohort of Mouse Knockouts within the International Mouse Phenotyping Consortium. Metabolites, 2019, 9, 101.	2.9	40
18	Systematic Error Removal Using Random Forest for Normalizing Large-Scale Untargeted Lipidomics Data. Analytical Chemistry, 2019, 91, 3590-3596.	6.5	163

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19	Structure Annotation of All Mass Spectra in Untargeted Metabolomics. Analytical Chemistry, 2019, 91, 2155-2162.	6.5	131
20	Identification of small molecules using accurate mass MS/MS search. Mass Spectrometry Reviews, 2018, 37, 513-532.	5.4	292
21	Identifying metabolites by integrating metabolome databases with mass spectrometry cheminformatics. Nature Methods, 2018, 15, 53-56.	19.0	368
22	Software Tools and Approaches for Compound Identification of LC-MS/MS Data in Metabolomics. Metabolites, 2018, 8, 31.	2.9	461
23	Increasing Compound Identification Rates in Untargeted Lipidomics Research with Liquid Chromatography Drift Timeâ€“Ion Mobility Mass Spectrometry. Analytical Chemistry, 2018, 90, 10758-10764.	6.5	63
24	Using Accurate Mass Gas Chromatographyâ€“Mass Spectrometry with the MINE Database for Epimetabolite Annotation. Analytical Chemistry, 2017, 89, 10171-10180.	6.5	25
25	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	6.1	122
26	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.	6.1	80
27	Strategies for dereplication of natural compounds using high-resolution tandem mass spectrometry. Phytochemistry Letters, 2017, 21, 313-319.	1.2	26
28	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.	5.2	19
29	Interstitial Cystitis-Associated Urinary Metabolites Identified by Mass-Spectrometry Based Metabolomics Analysis. Scientific Reports, 2016, 6, 39227.	3.3	33
30	Changes in plasma metabolites and glucose homeostasis during omega-3 polyunsaturated fatty acid supplementation in women with polycystic ovary syndrome. BBA Clinical, 2016, 5, 179-185.	4.1	39
31	Hydrogen Rearrangement Rules: Computational MS/MS Fragmentation and Structure Elucidation Using MS-FINDER Software. Analytical Chemistry, 2016, 88, 7946-7958.	6.5	441
32	Environmental Tobacco Smoke Alters Metabolic Systems in Adult Rats. Chemical Research in Toxicology, 2016, 29, 1818-1827.	3.3	12
33	Cofactor symbiosis for enhanced algal growth, biofuel production, and wastewater treatment. Algal Research, 2016, 17, 308-315.	4.6	53
34	Ultrafast Polyphenol Metabolomics of Red Wines Using MicroLC-MS/MS. Journal of Agricultural and Food Chemistry, 2016, 64, 505-512.	5.2	31
35	A Large and Phylogenetically Diverse Class of Type 1 Opsins Lacking a Canonical Retinal Binding Site. PLoS ONE, 2016, 11, e0156543.	2.5	11
36	An in silico MS/MS library for automatic annotation of novel FAHFA lipids. Journal of Cheminformatics, 2015, 7, 53.	6.1	59

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37	Retention projection enables accurate calculation of liquid chromatographic retention times across labs and methods. Journal of Chromatography A, 2015, 1412, 43-51.	3.7	47
38	MS-DIAL: data-independent MS/MS deconvolution for comprehensive metabolome analysis. Nature Methods, 2015, 12, 523-526.	19.0	1,955
39	MINEs: open access databases of computationally predicted enzyme promiscuity products for untargeted metabolomics. Journal of Cheminformatics, 2015, 7, 44.	6.1	172
40	Informatics for improved algal taxonomic classification and research: A case study of UTEX 2341. Algal Research, 2015, 12, 545-549.	4.6	20
41	Lipidomic Analysis of Chlamydomonas reinhardtii under Nitrogen and Sulfur Deprivation. PLoS ONE, 2015, 10, e0137948.	2.5	51
42	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, 14-18.	1.3	10
43	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, 7275-7286.	3.7	48
44	LipidBlast Templates As Flexible Tools for Creating New in-Silico Tandem Mass Spectral Libraries. Analytical Chemistry, 2014, 86, 11024-11027.	6.5	52
45	MS2Analyzer: A Software for Small Molecule Substructure Annotations from Accurate Tandem Mass Spectra. Analytical Chemistry, 2014, 86, 10724-10731.	6.5	82
46	LipidBlast in silico tandem mass spectrometry database for lipid identification. Nature Methods, 2013, 10, 755-758.	19.0	783
47	Role of Squalene in the Organization of Monolayers Derived from Lipid Extracts of Halobacterium salinarum. Langmuir, 2013, 29, 7922-7930.	3.5	35
48	Advances in structure elucidation of small molecules using mass spectrometry. , 2013, , 129-166.		2
49	Analysis of Polar Lipids inChlamydomonas reinhardtiiUsing Nanoelectrospray Direct Infusion Method and Gas Chromatography and Mass Spectrometric Detection. Acta Chimica Sinica, 2013, 71, 663.	1.4	2
50	Induced Pluripotent Stem Cells Show Metabolomic Differences to Embryonic Stem Cells in Polyunsaturated Phosphatidylcholines and Primary Metabolism. PLoS ONE, 2012, 7, e46770.	2.5	68
51	Identification of Naturally Occurring Fatty Acids of the Myelin Sheath That Resolve Neuroinflammation. Science Translational Medicine, 2012, 4, 137ra73.	12.4	58
52	MetaMapp: mapping and visualizing metabolomic data by integrating information from biochemical pathways and chemical and mass spectral similarity. BMC Bioinformatics, 2012, 13, 99.	2.6	203
53	Pharmacogenetics Meets Metabolomics: Discovery of Tryptophan as a New Endogenous OCT2 Substrate Related to Metformin Disposition. PLoS ONE, 2012, 7, e36637.	2.5	43
54	Qualitative analysis of algal secretions with multiple mass spectrometric platforms. Journal of Chromatography A, 2012, 1244, 139-147.	3.7	65

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55	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, 5895-5902.	6.5	77
56	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.	2.6	27
57	Extending biochemical databases by metabolomic surveys.. Journal of Biological Chemistry, 2011, 286, 30244.	3.4	0
58	Extending Biochemical Databases by Metabolomic Surveys. Journal of Biological Chemistry, 2011, 286, 23637-23643.	3.4	67
59	Advances in structure elucidation of small molecules using mass spectrometry. Bioanalytical Reviews, 2010, 2, 23-60.	0.2	393
60	Hydrocarbon phenotyping of algal species using pyrolysis-gas chromatography mass spectrometry. BMC Biotechnology, 2010, 10, 40.	3.3	26
61	Determination of elemental compositions by gas chromatography/timeâ€ofâ€flight mass spectrometry using chemical and electron ionization. Rapid Communications in Mass Spectrometry, 2010, 24, 1172-1180.	1.5	55
62	The Chemical Translation Serviceâ€"a web-based tool to improve standardization of metabolomic reports. Bioinformatics, 2010, 26, 2647-2648.	4.1	117
63	What are the obstacles for an integrated system for comprehensive interpretation of cross-platform metabolic profile data?. Bioanalysis, 2009, 1, 1511-1514.	1.5	7
64	Software platform virtualization in chemistry research and university teaching. Journal of Cheminformatics, 2009, 1, 18.	6.1	5
65	FiehnLib: Mass Spectral and Retention Index Libraries for Metabolomics Based on Quadrupole and Time-of-Flight Gas Chromatography/Mass Spectrometry. Analytical Chemistry, 2009, 81, 10038-10048.	6.5	1,294
66	How Large Is the Metabolome? A Critical Analysis of Data Exchange Practices in Chemistry. PLoS ONE, 2009, 4, e5440.	2.5	104
67	Quality control for plant metabolomics: reporting MSIâ€compliant studies. Plant Journal, 2008, 53, 691-704.	5.7	591
68	Metabolite profiling of human colon carcinoma â€“ deregulation of TCA cycle and amino acid turnover. Molecular Cancer, 2008, 7, 72.	19.2	285
69	A comprehensive urinary metabolomic approach for identifying kidney cancer. Analytical Biochemistry, 2007, 363, 185-195.	2.4	427
70	Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry. BMC Bioinformatics, 2007, 8, 105.	2.6	929
71	Metabolite Profiling in Blood Plasma. Methods in Molecular Biology, 2007, 358, 3-17.	0.9	101
72	Mass Spectrometryâ€"Based Metabolic Profiling Reveals Different Metabolite Patterns in Invasive Ovarian Carcinomas and Ovarian Borderline Tumors. Cancer Research, 2006, 66, 10795-10804.	0.9	366

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73	Metabolomic database annotations via query of elemental compositions: mass accuracy is insufficient even at less than 1 ppm. BMC Bioinformatics, 2006, 7, 234.	2.6	532
74	Use of boiling pointâ€“Lee retention index correlation for rapid review of gas chromatography-mass spectrometry data. Analytica Chimica Acta, 2003, 494, 235-243.	5.4	34
75	Sequential fractionation procedure for the identification of potentially cytochrome P4501A-inducing compounds. Journal of Chromatography A, 2003, 986, 55-66.	3.7	43
76	Erratum to â€œSequential fractionation procedure for the identification of potentially cytochrome P4501A-inducing compoundsâ€. Journal of Chromatography A, 2003, 993, 223.	3.7	0
77	Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. Environmental Pollution, 2003, 121, 81-85.	7.5	55
78	Effectâ€directed fractionation and identification of cytochrome P4501Aâ€inducing halogenated aromatic hydrocarbons in a contaminated sediment. Environmental Toxicology and Chemistry, 2002, 21, 2654-2662.	4.3	66