Justin J J Van Der Hooft

List of Publications by Year
in descending order

89 papers	18,857 citations	66234 42 h-index	60497 81 g-index
123 all docs	123 docs citations	123 times ranked	21770 citing authors

#	Article	IF	Citations
1	Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2. Nature Biotechnology, 2019, 37, 852-857.	9.4	11,167
2	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	9.0	650
3	The food metabolome: a window over dietary exposure. American Journal of Clinical Nutrition, 2014, 99, 1286-1308.	2.2	411
4	MIBiG 2.0: a repository for biosynthetic gene clusters of known function. Nucleic Acids Research, 2020, 48, D454-D458.	6.5	351
5	Reproducible molecular networking of untargeted mass spectrometry data using GNPS. Nature Protocols, 2020, 15, 1954-1991.	5.5	344
6	Topic modeling for untargeted substructure exploration in metabolomics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13738-13743.	3.3	269
7	The Natural Products Atlas: An Open Access Knowledge Base for Microbial Natural Products Discovery. ACS Central Science, 2019, 5, 1824-1833.	5.3	258
8	MolNetEnhancer: Enhanced Molecular Networks by Integrating Metabolome Mining and Annotation Tools. Metabolites, 2019, 9, 144.	1.3	245
9	Propagating annotations of molecular networks using in silico fragmentation. PLoS Computational Biology, 2018, 14, e1006089.	1.5	242
10	Human studies on the absorption, distribution, metabolism, and excretion of tea polyphenols. American Journal of Clinical Nutrition, 2013, 98, 1619S-1630S.	2.2	192
11	Accelerating Metabolite Identification in Natural Product Research: Toward an Ideal Combination of Liquid Chromatographyâ€“High-Resolution Tandem Mass Spectrometry and NMR Profiling, in Silico Databases, and Chemometrics. Analytical Chemistry, 2019, 91, 704-742.	3.2	165
12	Mass spectrometry searches using MASST. Nature Biotechnology, 2020, 38, 23-26.	9.4	160
13	Orange juice (poly)phenols are highly bioavailable in humans. American Journal of Clinical Nutrition, 2014, 100, 1378-1384.	2.2	133
14	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products. Journal of Natural Products, 2021, 84, 2795-2807.	1.5	131
15	Structural Elucidation and Quantification of Phenolic Conjugates Present in Human Urine after Tea Intake. Analytical Chemistry, 2012, 84, 7263-7271.	3.2	117
16	Substructureâ€based annotation of highâ€resolution multistage MSⁿ spectral trees. Rapid Communications in Mass Spectrometry, 2012, 26, 2461-2471.	0.7	117
17	Linking genomics and metabolomics to chart specialized metabolic diversity. Chemical Society Reviews, 2020, 49, 3297-3314.	18.7	114
18	Absorption, metabolism, distribution and excretion of (â^')-epicatechin: A review of recent findings. Molecular Aspects of Medicine, 2018, 61, 18-30.	2.7	113

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19	Updates in metabolomics tools and resources: 2014â€“2015. Electrophoresis, 2016, 37, 86-110.	1.3	110
20	NON-SMOKY GLYCOSYLTRANSFERASE1 Prevents the Release of Smoky Aroma from Tomato Fruit. Plant Cell, 2013, 25, 3067-3078.	3.1	108
21	Automatic Chemical Structure Annotation of an LCâ€“MSⁿ Based Metabolic Profile from Green Tea. Analytical Chemistry, 2013, 85, 6033-6040.	3.2	107
22	BiG-SLiCE: A highly scalable tool maps the diversity of 1.2 million biosynthetic gene clusters. GigaScience, 2021, 10, .	3.3	98
23	Polyphenol Identification Based on Systematic and Robust High-Resolution Accurate Mass Spectrometry Fragmentation. Analytical Chemistry, 2011, 83, 409-416.	3.2	94
24	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships. PLoS Computational Biology, 2021, 17, e1008724.	1.5	92
25	Interactions of black tea polyphenols with human gut microbiota: implications for gut and cardiovascular health. American Journal of Clinical Nutrition, 2013, 98, 1631S-1641S.	2.2	86
26	Metabolite Identification Using Automated Comparison of High-Resolution Multistage Mass Spectral Trees. Analytical Chemistry, 2012, 84, 5524-5534.	3.2	82
27	A community resource for paired genomic and metabolomic data mining. Nature Chemical Biology, 2021, 17, 363-368.	3.9	81
28	Structural Annotation and Elucidation of Conjugated Phenolic Compounds in Black, Green, and White Tea Extracts. Journal of Agricultural and Food Chemistry, 2012, 60, 8841-8850.	2.4	80
29	ReDU: a framework to find and reanalyze public mass spectrometry data. Nature Methods, 2020, 17, 901-904.	9.0	79
30	Auto-deconvolution and molecular networking of gas chromatographyâ€“mass spectrometry data. Nature Biotechnology, 2021, 39, 169-173.	9.4	78
31	Advances in decomposing complex metabolite mixtures using substructure- and network-based computational metabolomics approaches. Natural Product Reports, 2021, 38, 1967-1993.	5.2	78
32	Rapid and Sustained Systemic Circulation of Conjugated Gut Microbial Catabolites after Single-Dose Black Tea Extract Consumption. Journal of Proteome Research, 2014, 13, 2668-2678.	1.8	77
33	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. Nature Chemical Biology, 2021, 17, 146-151.	3.9	73
34	Ms2lda.org: web-based topic modelling for substructure discovery in mass spectrometry. Bioinformatics, 2018, 34, 317-318.	1.8	69
35	Automatic Compound Annotation from Mass Spectrometry Data Using MAGMa. Mass Spectrometry, 2014, 3, S0033-S0033.	0.2	66
36	Spectral trees as a robust annotation tool in LCâ€“MS based metabolomics. Metabolomics, 2012, 8, 691-703.	1.4	63

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37	Comprehensive mass spectrometryâ€guided phenotyping of plant specialized metabolites reveals metabolic diversity in the cosmopolitan plant family Rhamnaceae. Plant Journal, 2019, 98, 1134-1144.	2.8	59
38	Deciphering complex metabolite mixtures by unsupervised and supervised substructure discovery and semi-automated annotation from MS/MS spectra. Faraday Discussions, 2019, 218, 284-302.	1.6	55
39	Unsupervised Discovery and Comparison of Structural Families Across Multiple Samples in Untargeted Metabolomics. Analytical Chemistry, 2017, 89, 7569-7577.	3.2	52
40	Untargeted mass spectrometry-based metabolomics approach unveils molecular changes in raw and processed foods and beverages. Food Chemistry, 2020, 302, 125290.	4.2	52
41	A strategy for fast structural elucidation of metabolites in small volume plant extracts using automated MSâ€guided LCâ€MSâ€SPEâ€NMR. Magnetic Resonance in Chemistry, 2011, 49, S55-60.	1.1	51
42	MS2DeepScore: a novel deep learning similarity measure to compare tandem mass spectra. Journal of Cheminformatics, 2021, 13, 84.	2.8	51
43	matchms - processing and similarity evaluation of mass spectrometry data.. Journal of Open Source Software, 2020, 5, 2411.	2.0	48
44	Microbiome-derived carnitine mimics as previously unknown mediators of gut-brain axis communication. Science Advances, 2020, 6, eaax6328.	4.7	45
45	Structural elucidation of low abundant metabolites in complex sample matrices. Metabolomics, 2013, 9, 1009-1018.	1.4	42
46	A comprehensive evaluation of the [2- 14 C](â€“)-epicatechin metabolome in rats. Free Radical Biology and Medicine, 2016, 99, 128-138.	1.3	40
47	Assessing Specialized Metabolite Diversity in the Cosmopolitan Plant Genus Euphorbia L.. Frontiers in Plant Science, 2019, 10, 846.	1.7	40
48	In Silico Prediction and Automatic LCâ€“MSⁿ Annotation of Green Tea Metabolites in Urine. Analytical Chemistry, 2014, 86, 4767-4774.	3.2	39
49	Advancements in capturing and mining mass spectrometry data are transforming natural products research. Natural Product Reports, 2021, 38, 2066-2082.	5.2	38
50	Rapid Development of Improved Data-Dependent Acquisition Strategies. Analytical Chemistry, 2021, 93, 5676-5683.	3.2	31
51	Urinary antihypertensive drug metabolite screening using molecular networking coupled to high-resolution mass spectrometry fragmentation. Metabolomics, 2016, 12, 125.	1.4	30
52	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions. PLoS Computational Biology, 2021, 17, e1008920.	1.5	30
53	Unexpected differential metabolic responses of Campylobacter jejuni to the abundant presence of glutamate and fucose. Metabolomics, 2018, 14, 144.	1.4	25
54	Comparative Metabologenomics Analysis of Polar Actinomycetes. Marine Drugs, 2021, 19, 103.	2.2	22

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55	Computational Metabolomics Tools Reveal Metabolic Reconfigurations Underlying the Effects of Biostimulant Seaweed Extracts on Maize Plants under Drought Stress Conditions. Metabolites, 2022, 12, 487.	1.3	21
56	In Silico Optimization of Mass Spectrometry Fragmentation Strategies in Metabolomics. Metabolites, 2019, 9, 219.	1.3	18
57	Substantial Extracellular Metabolic Differences Found Between Phylogenetically Closely Related Probiotic and Pathogenic Strains of Escherichia coli. Frontiers in Microbiology, 2019, 10, 252.	1.5	17
58	Enhanced Acylcarnitine Annotation in High-Resolution Mass Spectrometry Data: Fragmentation Analysis for the Classification and Annotation of Acylcarnitines. Frontiers in Bioengineering and Biotechnology, 2015, 3, 26.	2.0	16
59	Phenylpropane as an Alternative Dearomatizing Unit of Indoles: Discovery of Inaequalisines A and B Using Substructure-Informed Molecular Networking. Organic Letters, 2020, 22, 6077-6081.	2.4	16
60	BiG-MAP: an Automated Pipeline To Profile Metabolic Gene Cluster Abundance and Expression in Microbiomes. MSystems, 2021, 6, e0093721.	1.7	16
61	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. PLoS Pathogens, 2020, 16, e1008932.	2.1	16
62	Identification of a drimenol synthase and drimenol oxidase from Persicaria hydropiper, involved in the biosynthesis of insect deterrent drimanes. Plant Journal, 2017, 90, 1052-1063.	2.8	15
63	Comprehensive Large-Scale Integrative Analysis of Omics Data To Accelerate Specialized Metabolite Discovery. MSystems, 2021, 6, e0072621.	1.7	15
64	Fungi population metabolomics and molecular network study reveal novel biomarkers for early detection of aflatoxigenic Aspergillus species. Journal of Hazardous Materials, 2022, 424, 127173.	6.5	15
65	Assessing specialized metabolite diversity of Alnus species by a digitized LCâ€“MS/MS data analysis workflow. Phytochemistry, 2020, 173, 112292.	1.4	15
66	Ranking Metabolite Sets by Their Activity Levels. Metabolites, 2021, 11, 103.	1.3	14
67	Thermal diffusivity of periderm from tomatoes of different maturity stages as determined by the concept of the frequency-domain open photoacoustic cell. Journal of Applied Physics, 2011, 109, .	1.1	13
68	Metabolomics-Guided Elucidation of Plant Abiotic Stress Responses in the 4IR Era: An Overview. Metabolites, 2021, 11, 445.	1.3	11
69	Iridoid and caffeoyl phenylethanoid glycosides of the endangered carnivorous plant Pinguicula lusitanica L. (Lentibulariaceae). Biochemical Systematics and Ecology, 2009, 37, 285-289.	0.6	9
70	An isotopic labeling approach linking natural products with biosynthetic gene clusters. Nature Chemical Biology, 2022, 18, 295-304.	3.9	9
71	A genetical metabolomics approach for bioprospecting plant biosynthetic gene clusters. BMC Research Notes, 2019, 12, 194.	0.6	7
72	Mass Spectral Molecular Networking to Profile the Metabolome of Biostimulant Bacillus Strains. Frontiers in Plant Science, 0, 13, .	1.7	7

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73	Inhibitory activity of plumbagin produced by Drosera intermedia on food spoilage fungi. Journal of the Science of Food and Agriculture, 2012, 92, 1638-1642.	1.7	6
74	Metabolic interactions shape a community's phenotype. Trends in Microbiology, 2022, 30, 609-611.	3.5	6
75	High resolution techniques: general discussion. Faraday Discussions, 2019, 218, 247-267.	1.6	4
76	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. Journal of Cheminformatics, 2021, 13, 64.	2.8	3
77	The Large Scale Identification and Quantification of Conjugates of Intact and Gut Microbial Bioconversion Products of Polyphenols. Special Publication - Royal Society of Chemistry, 2013, , 177-182.	0.0	2
78	Data mining and visualisation: general discussion. Faraday Discussions, 2019, 218, 354-371.	1.6	2
79	The Metabolomics Societyâ€"Current State of the Membership and Future Directions. Metabolites, 2019, 9, 89.	1.3	2
80	Chemical Gradients of Plant Substrates in an Atta texana Fungus Garden. MSystems, 2021, 6, e0060121.	1.7	2
81	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy. , 2017, , 1-33.		2
82	Future challenges and new approaches: general discussion. Faraday Discussions, 2019, 218, 505-523.	1.6	1
83	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy. , 2016, , 1-32.		1
84	Activity update from the early career members network. Metabolomics, 2015, 11, 247-248.	1.4	0
85	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy. , 2018, , 1309-1341.		0
86	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. , 2020, 16, e1008932.		0
87	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. , 2020, 16, e1008932.		0
88	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. , 2020, 16, e1008932.		0
89	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. , 2020, 16, e1008932.		0