

# Justin J J Van Der Hooft

## List of Publications by Citations

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103  
papers

8,235  
citations

36  
h-index

90  
g-index

123  
ext. papers

13,804  
ext. citations

9.4  
avg, IF

5.76  
L-index

#	Paper	IF	Citations
103	Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2. <i>Nature Biotechnology</i> , <b>2019</b> , 37, 852-857	44.5	4050
102	The food metabolome: a window over dietary exposure. <i>American Journal of Clinical Nutrition</i> , <b>2014</b> , 99, 1286-308	7	335
101	Feature-based molecular networking in the GNPS analysis environment. <i>Nature Methods</i> , <b>2020</b> , 17, 905-908	20.8	207
100	MIBiG 2.0: a repository for biosynthetic gene clusters of known function. <i>Nucleic Acids Research</i> , <b>2020</b> , 48, D454-D458	20.1	180
99	Human studies on the absorption, distribution, metabolism, and excretion of tea polyphenols. <i>American Journal of Clinical Nutrition</i> , <b>2013</b> , 98, 1619S-1630S	7	165
98	Topic modeling for untargeted substructure exploration in metabolomics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, 13738-13743	11.5	163
97	Propagating annotations of molecular networks using in silico fragmentation. <i>PLoS Computational Biology</i> , <b>2018</b> , 14, e1006089	5	139
96	QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science		138
95	The Natural Products Atlas: An Open Access Knowledge Base for Microbial Natural Products Discovery. <i>ACS Central Science</i> , <b>2019</b> , 5, 1824-1833	16.8	137
94	Reproducible molecular networking of untargeted mass spectrometry data using GNPS. <i>Nature Protocols</i> , <b>2020</b> , 15, 1954-1991	18.8	125
93	Orange juice (poly)phenols are highly bioavailable in humans. <i>American Journal of Clinical Nutrition</i> , <b>2014</b> , 100, 1378-84	7	104
92	Updates in metabolomics tools and resources: 2014-2015. <i>Electrophoresis</i> , <b>2016</b> , 37, 86-110	3.6	102
91	MolNetEnhancer: Enhanced Molecular Networks by Integrating Metabolome Mining and Annotation Tools. <i>Metabolites</i> , <b>2019</b> , 9,	5.6	101
90	Structural elucidation and quantification of phenolic conjugates present in human urine after tea intake. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 7263-71	7.8	101
89	Accelerating Metabolite Identification in Natural Product Research: Toward an Ideal Combination of Liquid Chromatography-High-Resolution Tandem Mass Spectrometry and NMR Profiling, in Silico Databases, and Chemometrics. <i>Analytical Chemistry</i> , <b>2019</b> , 91, 704-742	7.8	101
88	Substructure-based annotation of high-resolution multistage MS(n) spectral trees. <i>Rapid Communications in Mass Spectrometry</i> , <b>2012</b> , 26, 2461-71	2.2	99
87	Polyphenol identification based on systematic and robust high-resolution accurate mass spectrometry fragmentation. <i>Analytical Chemistry</i> , <b>2011</b> , 83, 409-16	7.8	92

86	Automatic chemical structure annotation of an LC-MS(n) based metabolic profile from green tea. <i>Analytical Chemistry</i> , <b>2013</b> , 85, 6033-40	7.8	88
85	Metabolite identification using automated comparison of high-resolution multistage mass spectral trees. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 5524-34	7.8	79
84	QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science <b>2018</b> ,		78
83	Absorption, metabolism, distribution and excretion of (-)-epicatechin: A review of recent findings. <i>Molecular Aspects of Medicine</i> , <b>2018</b> , 61, 18-30	16.7	76
82	Mass spectrometry searches using MASST. <i>Nature Biotechnology</i> , <b>2020</b> , 38, 23-26	44.5	74
81	Interactions of black tea polyphenols with human gut microbiota: implications for gut and cardiovascular health. <i>American Journal of Clinical Nutrition</i> , <b>2013</b> , 98, 1631S-1641S	7	73
80	Structural annotation and elucidation of conjugated phenolic compounds in black, green, and white tea extracts. <i>Journal of Agricultural and Food Chemistry</i> , <b>2012</b> , 60, 8841-50	5.7	69
79	Non-smoky glycosyltransferase1 prevents the release of smoky aroma from tomato fruit. <i>Plant Cell</i> , <b>2013</b> , 25, 3067-78	11.6	64
78	Spectral trees as a robust annotation tool in LCMS based metabolomics. <i>Metabolomics</i> , <b>2012</b> , 8, 691-703	4.7	59
77	Rapid and sustained systemic circulation of conjugated gut microbial catabolites after single-dose black tea extract consumption. <i>Journal of Proteome Research</i> , <b>2014</b> , 13, 2668-78	5.6	57
76	Linking genomics and metabolomics to chart specialized metabolic diversity. <i>Chemical Society Reviews</i> , <b>2020</b> , 49, 3297-3314	58.5	52
75	Automatic Compound Annotation from Mass Spectrometry Data Using MAGMa. <i>Mass Spectrometry</i> , <b>2014</b> , 3, S0033	1.7	50
74	A strategy for fast structural elucidation of metabolites in small volume plant extracts using automated MS-guided LC-MS-SPE-NMR. <i>Magnetic Resonance in Chemistry</i> , <b>2011</b> , 49 Suppl 1, S55-60	2.1	46
73	Ms2lda.org: web-based topic modelling for substructure discovery in mass spectrometry. <i>Bioinformatics</i> , <b>2018</b> , 34, 317-318	7.2	41
72	Structural elucidation of low abundant metabolites in complex sample matrices. <i>Metabolomics</i> , <b>2013</b> , 9, 1009-1018	4.7	41
71	QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science		36
70	A comprehensive evaluation of the [2-C](-)-epicatechin metabolome in rats. <i>Free Radical Biology and Medicine</i> , <b>2016</b> , 99, 128-138	7.8	36
69	Auto-deconvolution and molecular networking of gas chromatography-mass spectrometry data. <i>Nature Biotechnology</i> , <b>2021</b> , 39, 169-173	44.5	36

68	In silico prediction and automatic LC-MS(n) annotation of green tea metabolites in urine. <i>Analytical Chemistry</i> , <b>2014</b> , 86, 4767-74	7.8	35
67	Untargeted mass spectrometry-based metabolomics approach unveils molecular changes in raw and processed foods and beverages. <i>Food Chemistry</i> , <b>2020</b> , 302, 125290	8.5	34
66	Unsupervised Discovery and Comparison of Structural Families Across Multiple Samples in Untargeted Metabolomics. <i>Analytical Chemistry</i> , <b>2017</b> , 89, 7569-7577	7.8	33
65	Comprehensive mass spectrometry-guided phenotyping of plant specialized metabolites reveals metabolic diversity in the cosmopolitan plant family Rhamnaceae. <i>Plant Journal</i> , <b>2019</b> , 98, 1134-1144	6.9	32
64	A community resource for paired genomic and metabolomic data mining. <i>Nature Chemical Biology</i> , <b>2021</b> , 17, 363-368	11.7	32
63	BiG-SLiCE: A highly scalable tool maps the diversity of 1.2 million biosynthetic gene clusters. <i>GigaScience</i> , <b>2021</b> , 10,	7.6	30
62	Feature-based Molecular Networking in the GNPS Analysis Environment		29
61	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. <i>Nature Chemical Biology</i> , <b>2021</b> , 17, 146-151	11.7	29
60	Deciphering complex metabolite mixtures by unsupervised and supervised substructure discovery and semi-automated annotation from MS/MS spectra. <i>Faraday Discussions</i> , <b>2019</b> , 218, 284-302	3.6	28
59	ReDU: a framework to find and reanalyze public mass spectrometry data. <i>Nature Methods</i> , <b>2020</b> , 17, 901-904	10.4	28
58	Assessing Specialized Metabolite Diversity in the Cosmopolitan Plant Genus L. <i>Frontiers in Plant Science</i> , <b>2019</b> , 10, 846	6.2	27
57	Microbiome-derived carnitine mimics as previously unknown mediators of gut-brain axis communication. <i>Science Advances</i> , <b>2020</b> , 6, eaax6328	14.3	24
56	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships. <i>PLoS Computational Biology</i> , <b>2021</b> , 17, e1008724	5	24
55	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products. <i>Journal of Natural Products</i> , <b>2021</b> , 84, 2795-2807	4.9	21
54	Urinary antihypertensive drug metabolite screening using molecular networking coupled to high-resolution mass spectrometry fragmentation. <i>Metabolomics</i> , <b>2016</b> , 12, 125	4.7	17
53	Repository-scale Co- and Re-analysis of Tandem Mass Spectrometry Data		14
52	Enhanced acylcarnitine annotation in high-resolution mass spectrometry data: fragmentation analysis for the classification and annotation of acylcarnitines. <i>Frontiers in Bioengineering and Biotechnology</i> , <b>2015</b> , 3, 26	5.8	13
51	Unexpected differential metabolic responses of <i>Campylobacter jejuni</i> to the abundant presence of glutamate and fucose. <i>Metabolomics</i> , <b>2018</b> , 14, 144	4.7	13

50	Advances in decomposing complex metabolite mixtures using substructure- and network-based computational metabolomics approaches. <i>Natural Product Reports</i> , <b>2021</b> , 38, 1967-1993	15.1	11
49	MolNetEnhancer: enhanced molecular networks by integrating metabolome mining and annotation tools		10
48	Rapid Development of Improved Data-Dependent Acquisition Strategies. <i>Analytical Chemistry</i> , <b>2021</b> , 93, 5676-5683	7.8	10
47	In Silico Optimization of Mass Spectrometry Fragmentation Strategies in Metabolomics. <i>Metabolites</i> , <b>2019</b> , 9,	5.6	9
46	Iridoid and caffeoyl phenylethanoid glycosides of the endangered carnivorous plant <i>Pinguicula lusitanica</i> L. (Lentibulariaceae). <i>Biochemical Systematics and Ecology</i> , <b>2009</b> , 37, 285-289	1.4	9
45	Thermal diffusivity of periderm from tomatoes of different maturity stages as determined by the concept of the frequency-domain open photoacoustic cell. <i>Journal of Applied Physics</i> , <b>2011</b> , 109, 034703 <sup>2.5</sup>		9
44	matchms - processing and similarity evaluation of mass spectrometry data.. <i>Journal of Open Source Software</i> , <b>2020</b> , 5, 2411	5.2	9
43	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products		9
42	Assessing specialized metabolite diversity of <i>Alnus</i> species by a digitized LC-MS/MS data analysis workflow. <i>Phytochemistry</i> , <b>2020</b> , 173, 112292	4	9
41	Phenylpropane as an Alternative Dearomatizing Unit of Indoles: Discovery of Inaequalisines A and B Using Substructure-Informed Molecular Networking. <i>Organic Letters</i> , <b>2020</b> , 22, 6077-6081	6.2	9
40	Identification of a drimenol synthase and drimenol oxidase from <i>Persicaria hydropiper</i> , involved in the biosynthesis of insect deterrent drimanes. <i>Plant Journal</i> , <b>2017</b> , 90, 1052-1063	6.9	8
39	Substantial Extracellular Metabolic Differences Found Between Phylogenetically Closely Related Probiotic and Pathogenic Strains of. <i>Frontiers in Microbiology</i> , <b>2019</b> , 10, 252	5.7	8
38	MS2DeepScore: a novel deep learning similarity measure to compare tandem mass spectra. <i>Journal of Cheminformatics</i> , <b>2021</b> , 13, 84	8.6	8
37	MASST: A Web-based Basic Mass Spectrometry Search Tool for Molecules to Search Public Data		8
36	Reproducible Molecular Networking Of Untargeted Mass Spectrometry Data Using GNPS.		7
35	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions. <i>PLoS Computational Biology</i> , <b>2021</b> , 17, e1008920	5	7
34	Comparative Metabologenomics Analysis of Polar Actinomycetes. <i>Marine Drugs</i> , <b>2021</b> , 19,	6	7
33	Inhibitory activity of plumbagin produced by <i>Drosera intermedia</i> on food spoilage fungi. <i>Journal of the Science of Food and Agriculture</i> , <b>2012</b> , 92, 1638-42	4.3	6

32	Advancements in capturing and mining mass spectrometry data are transforming natural products research. <i>Natural Product Reports</i> , <b>2021</b> , 38, 2066-2082	15.1	6
31	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions		6
30	BiG-SLiCE: A Highly Scalable Tool Maps the Diversity of 1.2 Million Biosynthetic Gene Clusters		6
29	Ranking Metabolite Sets by Their Activity Levels. <i>Metabolites</i> , <b>2021</b> , 11,	5.6	6
28	A genetical metabolomics approach for bioprospecting plant biosynthetic gene clusters. <i>BMC Research Notes</i> , <b>2019</b> , 12, 194	2.3	5
27	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. <i>PLoS Pathogens</i> , <b>2020</b> , 16, e1008932	7.6	5
26	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships		5
25	Decomposing metabolite set activity levels with PALS		4
24	BiG-MAP: an automated pipeline to profile metabolic gene cluster abundance and expression in microbiomes		4
23	Did a plant-herbivore arms race drive chemical diversity in Euphorbia?		4
22	MS2DeepScore - a novel deep learning similarity measure for mass fragmentation spectrum comparisons		4
21	High resolution techniques: general discussion. <i>Faraday Discussions</i> , <b>2019</b> , 218, 247-267	3.6	3
20	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products		3
19	Chemically-informed Analyses of Metabolomics Mass Spectrometry Data with Qemistree		3
18	Comprehensive Large-Scale Integrative Analysis of Omics Data To Accelerate Specialized Metabolite Discovery. <i>MSystems</i> , <b>2021</b> , 6, e0072621	7.6	3
17	Fungi population metabolomics and molecular network study reveal novel biomarkers for early detection of aflatoxigenic <i>Aspergillus</i> species. <i>Journal of Hazardous Materials</i> , <b>2022</b> , 424, 127173	12.8	3
16	Data mining and visualisation: general discussion. <i>Faraday Discussions</i> , <b>2019</b> , 218, 354-371	3.6	2
15	The Large Scale Identification and Quantification of Conjugates of Intact and Gut Microbial Bioconversion Products of Polyphenols. <i>Special Publication - Royal Society of Chemistry</i> , <b>2013</b> , 177-182	0.1	2

14	In-silico Optimisation of Mass Spectrometry Fragmentation Strategies in Metabolomics		2
13	Metabolomics-Guided Elucidation of Plant Abiotic Stress Responses in the 4IR Era: An Overview. <i>Metabolites</i> , <b>2021</b> , 11,	5.6	2
12	Computational Metabolomics Tools Reveal Metabolic Reconfigurations Underlying the Effects of Biostimulant Seaweed Extracts on Maize Plants under Drought Stress Conditions. <i>Metabolites</i> , <b>2022</b> , 12, 487	5.6	2
11	Implementations of the chemical structural and compositional similarity metric in R and Python		1
10	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy <b>2017</b> , 1-33		1
9	BiG-MAP: an Automated Pipeline To Profile Metabolic Gene Cluster Abundance and Expression in Microbiomes. <i>MSystems</i> , <b>2021</b> , 6, e0093721	7.6	1
8	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. <i>Journal of Cheminformatics</i> , <b>2021</b> , 13, 64	8.6	1
7	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy <b>2016</b> , 1-32		0
6	Chemical Gradients of Plant Substrates in an Fungus Garden. <i>MSystems</i> , <b>2021</b> , 6, e0060121	7.6	0
5	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy <b>2018</b> , 1309-1341		
4	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs <b>2020</b> , 16, e1008932		
3	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs <b>2020</b> , 16, e1008932		
2	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs <b>2020</b> , 16, e1008932		
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