Justin J J Van Der Hooft

List of Publications by Year in Descending Order

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	Fungi population metabolomics and molecular network study reveal novel biomarkers for early detection of aflatoxigenic Aspergillus species. *Journal of Hazardous Materials*, **2022**, 424, 127173	12.8	3
102	Computational Metabolomics Tools Reveal Metabolic Reconfigurations Underlying the Effects of Biostimulant Seaweed Extracts on Maize Plants under Drought Stress Conditions. *Metabolites*, **2022**, 12, 487	5.6	2
101	Advancements in capturing and mining mass spectrometry data are transforming natural products research. *Natural Product Reports*, **2021**, 38, 2066-2082	15.1	6
100	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products. *Journal of Natural Products*, **2021**, 84, 2795-2807	4.9	21
99	MS2DeepScore: a novel deep learning similarity measure to compare tandem mass spectra. *Journal of Cheminformatics*, **2021**, 13, 84	8.6	8
98	Rapid Development of Improved Data-Dependent Acquisition Strategies. *Analytical Chemistry*, **2021**, 93, 5676-5683	7.8	10
97	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions. *PLoS Computational Biology*, **2021**, 17, e1008920	5	7
96	Auto-deconvolution and molecular networking of gas chromatography-mass spectrometry data. *Nature Biotechnology*, **2021**, 39, 169-173	44.5	36
95	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. *Nature Chemical Biology*, **2021**, 17, 146-151	11.7	29
94	Advances in decomposing complex metabolite mixtures using substructure- and network-based computational metabolomics approaches. *Natural Product Reports*, **2021**, 38, 1967-1993	15.1	11
93	BiG-SLiCE: A highly scalable tool maps the diversity of 1.2 million biosynthetic gene clusters. *GigaScience*, **2021**, 10,	7.6	30
92	Ranking Metabolite Sets by Their Activity Levels. *Metabolites*, **2021**, 11,	5.6	6
91	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships. *PLoS Computational Biology*, **2021**, 17, e1008724	5	24
90	A community resource for paired genomic and metabolomic data mining. *Nature Chemical Biology*, **2021**, 17, 363-368	11.7	32
89	Comparative Metabologenomics Analysis of Polar Actinomycetes. *Marine Drugs*, **2021**, 19,	6	7
88	Metabolomics-Guided Elucidation of Plant Abiotic Stress Responses in the 4IR Era: An Overview. *Metabolites*, **2021**, 11,	5.6	2
87	Comprehensive Large-Scale Integrative Analysis of Omics Data To Accelerate Specialized Metabolite Discovery. *MSystems*, **2021**, 6, e0072621	7.6	3

86	Chemical Gradients of Plant Substrates in an Fungus Garden. *MSystems*, **2021**, 6, e0060121	7.6	0
85	BiG-MAP: an Automated Pipeline To Profile Metabolic Gene Cluster Abundance and Expression in Microbiomes. *MSystems*, **2021**, 6, e0093721	7.6	1
84	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. *Journal of Cheminformatics*, **2021**, 13, 64	8.6	1
83	Linking genomics and metabolomics to chart specialized metabolic diversity. *Chemical Society Reviews*, **2020**, 49, 3297-3314	58.5	52
82	Reproducible molecular networking of untargeted mass spectrometry data using GNPS. *Nature Protocols*, **2020**, 15, 1954-1991	18.8	125
81	Microbiome-derived carnitine mimics as previously unknown mediators of gut-brain axis communication. *Science Advances*, **2020**, 6, eaax6328	14.3	24
80	MIBiG 2.0: a repository for biosynthetic gene clusters of known function. *Nucleic Acids Research*, **2020**, 48, D454-D458	20.1	180
79	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs. *PLoS Pathogens*, **2020**, 16, e1008932	7.6	5
78	matchms - processing and similarity evaluation of mass spectrometry data.. *Journal of Open Source Software*, **2020**, 5, 2411	5.2	9
77	Assessing specialized metabolite diversity of Alnus species by a digitized LC-MS/MS data analysis workflow. *Phytochemistry*, **2020**, 173, 112292	4	9
76	Mass spectrometry searches using MASST. *Nature Biotechnology*, **2020**, 38, 23-26	44.5	74
75	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	6.2	9
74	Feature-based molecular networking in the GNPS analysis environment. *Nature Methods*, **2020**, 17, 905-908	28.6	207
73	ReDU: a framework to find and reanalyze public mass spectrometry data. *Nature Methods*, **2020**, 17, 901-904	28.6	28
72	Untargeted mass spectrometry-based metabolomics approach unveils molecular changes in raw and processed foods and beverages. *Food Chemistry*, **2020**, 302, 125290	8.5	34
71	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs **2020**, 16, e1008932		
70	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs **2020**, 16, e1008932		
69	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs **2020**, 16, e1008932		

68	Veterinary trypanocidal benzoxaboroles are peptidase-activated prodrugs **2020**, 16, e1008932		
67	Deciphering complex metabolite mixtures by unsupervised and supervised substructure discovery and semi-automated annotation from MS/MS spectra. *Faraday Discussions*, **2019**, 218, 284-302	3.6	28
66	Substantial Extracellular Metabolic Differences Found Between Phylogenetically Closely Related Probiotic and Pathogenic Strains of. *Frontiers in Microbiology*, **2019**, 10, 252	5.7	8
65	A genetical metabolomics approach for bioprospecting plant biosynthetic gene clusters. *BMC Research Notes*, **2019**, 12, 194	2.3	5
64	High resolution techniques: general discussion. *Faraday Discussions*, **2019**, 218, 247-267	3.6	3
63	Data mining and visualisation: general discussion. *Faraday Discussions*, **2019**, 218, 354-371	3.6	2
62	MolNetEnhancer: Enhanced Molecular Networks by Integrating Metabolome Mining and Annotation Tools. *Metabolites*, **2019**, 9,	5.6	101
61	Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2. *Nature Biotechnology*, **2019**, 37, 852-857	44.5	4050
60	Assessing Specialized Metabolite Diversity in the Cosmopolitan Plant Genus L. *Frontiers in Plant Science*, **2019**, 10, 846	6.2	27
59	In Silico Optimization of Mass Spectrometry Fragmentation Strategies in Metabolomics. *Metabolites*, **2019**, 9,	5.6	9
58	The Natural Products Atlas: An Open Access Knowledge Base for Microbial Natural Products Discovery. *ACS Central Science*, **2019**, 5, 1824-1833	16.8	137
57	Comprehensive mass spectrometry-guided phenotyping of plant specialized metabolites reveals metabolic diversity in the cosmopolitan plant family Rhamnaceae. *Plant Journal*, **2019**, 98, 1134-1144	6.9	32
56	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. *Analytical Chemistry*, **2019**, 91, 704-742	7.8	101
55	Ms2lda.org: web-based topic modelling for substructure discovery in mass spectrometry. *Bioinformatics*, **2018**, 34, 317-318	7.2	41
54	QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science **2018**,		78
53	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy **2018**, 1309-1341		
52	Absorption, metabolism, distribution and excretion of (-)-epicatechin: A review of recent findings. *Molecular Aspects of Medicine*, **2018**, 61, 18-30	16.7	76
51	Unexpected differential metabolic responses of Campylobacter jejuni to the abundant presence of glutamate and fucose. *Metabolomics*, **2018**, 14, 144	4.7	13

50	Propagating annotations of molecular networks using in silico fragmentation. *PLoS Computational Biology*, **2018**, 14, e1006089	5	139
49	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	6.9	8
48	Unsupervised Discovery and Comparison of Structural Families Across Multiple Samples in Untargeted Metabolomics. *Analytical Chemistry*, **2017**, 89, 7569-7577	7.8	33
47	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy **2017**, 1-33		1
46	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	11.5	163
45	Metabolite Identification in Complex Mixtures Using Nuclear Magnetic Resonance Spectroscopy **2016**, 1-32		0
44	Urinary antihypertensive drug metabolite screening using molecular networking coupled to high-resolution mass spectrometry fragmentation. *Metabolomics*, **2016**, 12, 125	4.7	17
43	Updates in metabolomics tools and resources: 2014-2015. *Electrophoresis*, **2016**, 37, 86-110	3.6	102
42	A comprehensive evaluation of the [2-C](-)-epicatechin metabolome in rats. *Free Radical Biology and Medicine*, **2016**, 99, 128-138	7.8	36
41	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	5.8	13
40	The food metabolome: a window over dietary exposure. *American Journal of Clinical Nutrition*, **2014** , 99, 1286-308	7	335
39	In silico prediction and automatic LC-MS(n) annotation of green tea metabolites in urine. *Analytical Chemistry*, **2014**, 86, 4767-74	7.8	35
38	Rapid and sustained systemic circulation of conjugated gut microbial catabolites after single-dose black tea extract consumption. *Journal of Proteome Research*, **2014**, 13, 2668-78	5.6	57
37	Automatic Compound Annotation from Mass Spectrometry Data Using MAGMa. *Mass Spectrometry*, **2014**, 3, S0033	1.7	50
36	Orange juice (poly)phenols are highly bioavailable in humans. *American Journal of Clinical Nutrition*, **2014**, 100, 1378-84	7	104
35	Structural elucidation of low abundant metabolites in complex sample matrices. *Metabolomics*, **2013**, 9, 1009-1018	4.7	41
34	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	0.1	2
33	Automatic chemical structure annotation of an LC-MS(n) based metabolic profile from green tea. *Analytical Chemistry*, **2013**, 85, 6033-40	7.8	88

32	Human studies on the absorption, distribution, metabolism, and excretion of tea polyphenols. *American Journal of Clinical Nutrition*, **2013**, 98, 1619S-1630S	7	165
31	Non-smoky glycosyltransferase1 prevents the release of smoky aroma from tomato fruit. *Plant Cell*, **2013**, 25, 3067-78	11.6	64
30	Interactions of black tea polyphenols with human gut microbiota: implications for gut and cardiovascular health. *American Journal of Clinical Nutrition*, **2013**, 98, 1631S-1641S	7	73
29	Structural elucidation and quantification of phenolic conjugates present in human urine after tea intake. *Analytical Chemistry*, **2012**, 84, 7263-71	7.8	101
28	Metabolite identification using automated comparison of high-resolution multistage mass spectral trees. *Analytical Chemistry*, **2012**, 84, 5524-34	7.8	79
27	Structural annotation and elucidation of conjugated phenolic compounds in black, green, and white tea extracts. *Journal of Agricultural and Food Chemistry*, **2012**, 60, 8841-50	5.7	69
26	Substructure-based annotation of high-resolution multistage MS(n) spectral trees. *Rapid Communications in Mass Spectrometry*, **2012**, 26, 2461-71	2.2	99
25	Inhibitory activity of plumbagin produced by Drosera intermedia on food spoilage fungi. *Journal of the Science of Food and Agriculture*, **2012**, 92, 1638-42	4.3	6
24	Spectral trees as a robust annotation tool in LCMS based metabolomics. *Metabolomics*, **2012**, 8, 691-703	4.7	59
23	Polyphenol identification based on systematic and robust high-resolution accurate mass spectrometry fragmentation. *Analytical Chemistry*, **2011**, 83, 409-16	7.8	92
22	A strategy for fast structural elucidation of metabolites in small volume plant extracts using automated MS-guided LC-MS-SPE-NMR. *Magnetic Resonance in Chemistry*, **2011**, 49 Suppl 1, S55-60	2.1	46
21	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, 034703	2.5	9
20	Iridoid and caffeoyl phenylethanoid glycosides of the endangered carnivorous plant Pinguicula lusitanica L. (Lentibulariaceae). *Biochemical Systematics and Ecology*, **2009**, 37, 285-289	1.4	9
19	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products		3
18	NPClassifier: A Deep Neural Network-Based Structural Classification Tool for Natural Products		9
17	Reproducible Molecular Networking Of Untargeted Mass Spectrometry Data Using GNPS.		7
16	QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science		36
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