## Simon Rogers

List of Publications by Year in descending order

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SIMON POCEDS

#	Article	IF	CITATIONS
1	ViMMS 2.0: A framework to develop, test and optimise fragmentation strategies in LC-MS metabolomics. Journal of Open Source Software, 2022, 7, 3990.	4.6	5
2	Using topic modeling to detect cellular crosstalk in scRNA-seq. PLoS Computational Biology, 2022, 18, e1009975.	3.2	6
3	Gestational age-dependent development of the neonatal metabolome. Pediatric Research, 2021, 89, 1396-1404.	2.3	16
4	R package for statistical inference in dynamical systems using kernel based gradient matching: KGode. Computational Statistics, 2021, 36, 715-747.	1.5	0
5	Advances in decomposing complex metabolite mixtures using substructure- and network-based computational metabolomics approaches. Natural Product Reports, 2021, 38, 1967-1993.	10.3	78
6	Ranking Metabolite Sets by Their Activity Levels. Metabolites, 2021, 11, 103.	2.9	14
7	Spec2Vec: Improved mass spectral similarity scoring through learning of structural relationships. PLoS Computational Biology, 2021, 17, e1008724.	3.2	92
8	A community resource for paired genomic and metabolomic data mining. Nature Chemical Biology, 2021, 17, 363-368.	8.0	81
9	Comparative Metabologenomics Analysis of Polar Actinomycetes. Marine Drugs, 2021, 19, 103.	4.6	22
10	Up-down biphasic volume response of human red blood cells to PIEZO1 activation during capillary transits. PLoS Computational Biology, 2021, 17, e1008706.	3.2	17
11	PIEZO1 and the mechanism of the long circulatory longevity of human red blood cells. PLoS Computational Biology, 2021, 17, e1008496.	3.2	14
12	Rapid Development of Improved Data-Dependent Acquisition Strategies. Analytical Chemistry, 2021, 93, 5676-5683.	6.5	31
13	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions. PLoS Computational Biology, 2021, 17, e1008920.	3.2	30
14	Development and Validation of a Nonremission Risk Prediction Model in First-Episode Psychosis: An Analysis of 2 Longitudinal Studies. Schizophrenia Bulletin Open, 2021, 2, sgab041.	1.7	5
15	Probabilistic framework for integration of mass spectrum and retention time information in small molecule identification. Bioinformatics, 2021, 37, 1724-1731.	4.1	7
16	Feature-based molecular networking in the GNPS analysis environment. Nature Methods, 2020, 17, 905-908.	19.0	650
17	Predicting host taxonomic information from viral genomes: A comparison of feature representations. PLoS Computational Biology, 2020, 16, e1007894.	3.2	31
18	Towards development of a statistical framework to evaluate myotonic dystrophy type 1 mRNA biomarkers in the context of a clinical trial. PLoS ONE, 2020, 15, e0231000.	2.5	6

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19	matchms - processing and similarity evaluation of mass spectrometry data Journal of Open Source Software, 2020, 5, 2411.	4.6	48
20	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		0
21	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		0
22	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		0
23	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		0
24	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		0
25	Predicting host taxonomic information from viral genomes: A comparison of feature representations. , 2020, 16, e1007894.		1
26	Title is missing!. , 2020, 15, e0231000.		0
27	Title is missing!. , 2020, 15, e0231000.		0
28	Title is missing!. , 2020, 15, e0231000.		0
29	Title is missing!. , 2020, 15, e0231000.		0
30	Title is missing!. , 2020, 15, e0231000.		0
31	Title is missing!. , 2020, 15, e0231000.		0
32	Data mining and visualisation: general discussion. Faraday Discussions, 2019, 218, 354-371.	3.2	2
33	MolNetEnhancer: Enhanced Molecular Networks by Integrating Metabolome Mining and Annotation Tools. Metabolites, 2019, 9, 144.	2.9	245
34	Linking biosynthetic and chemical space to accelerate microbial secondary metabolite discovery. FEMS Microbiology Letters, 2019, 366, .	1.8	30
35	In Silico Optimization of Mass Spectrometry Fragmentation Strategies in Metabolomics. Metabolites, 2019, 9, 219.	2.9	18
36	Integrated Probabilistic Annotation: A Bayesian-Based Annotation Method for Metabolomic Profiles Integrating Biochemical Connections, Isotope Patterns, and Adduct Relationships. Analytical Chemistry, 2019, 91, 12799-12807.	6.5	17

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37	Deciphering complex metabolite mixtures by unsupervised and supervised substructure discovery and semi-automated annotation from MS/MS spectra. Faraday Discussions, 2019, 218, 284-302.	3.2	55
38	Statistical inference in mechanistic models: time warping for improved gradient matching. Computational Statistics, 2018, 33, 1091-1123.	1.5	1
39	Ms2lda.org: web-based topic modelling for substructure discovery in mass spectrometry. Bioinformatics, 2018, 34, 317-318.	4.1	69
40	Minimally-destructive atmospheric ionisation mass spectrometry authenticates authorship of historical manuscripts. Scientific Reports, 2018, 8, 10944.	3.3	6
41	EZ-Root-VIS: A Software Pipeline for the Rapid Analysis and Visual Reconstruction of Root System Architecture. Plant Physiology, 2018, 177, 1368-1381.	4.8	38
42	Global Sensitivity Analysis of OnGuard Models Identifies Key Hubs for Transport Interaction in Stomatal Dynamics. Plant Physiology, 2017, 174, 680-688.	4.8	23
43	Unsupervised Discovery and Comparison of Structural Families Across Multiple Samples in Untargeted Metabolomics. Analytical Chemistry, 2017, 89, 7569-7577.	6.5	52
44	PiMP my metabolome: an integrated, web-based tool for LC-MS metabolomics data. Bioinformatics, 2017, 33, 4007-4009.	4.1	41
45	Unexpected Connections between Humidity and Ion Transport Discovered Using a Model to Bridge Guard Cell-to-Leaf Scales. Plant Cell, 2017, 29, 2921-2939.	6.6	39
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.	7.1	269
47	An Optimal Frequency in Ca <sup>2+</sup> Oscillations for Stomatal Closure Is an Emergent Property of Ion Transport in Guard Cells. Plant Physiology, 2016, 170, 33-42.	4.8	51
48	Incorporating peak grouping information for alignment of multiple liquid chromatography-mass spectrometry datasets. Bioinformatics, 2015, 31, 1999-2006.	4.1	10
49	Stronger findings for metabolomics through Bayesian modeling of multiple peaks and compound correlations. Bioinformatics, 2014, 30, i461-i467.	4.1	8
50	MetAssign: probabilistic annotation of metabolites from LC–MS data using a Bayesian clustering approach. Bioinformatics, 2014, 30, 2764-2771.	4.1	63
51	Discrete and continuous time simulations of spatial ecological processes predict different final population sizes and interspecific competition outcomes. Ecological Modelling, 2013, 259, 50-61.	2.5	6
52	The Latent Process Decomposition of cDNA Microarray Data Sets. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2005, 2, 143-156.	3.0	66