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List of Publications by Year
in descending order

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77 papers	7,323 citations	218381 26 h-index	66788 78 g-index
80 all docs	80 docs citations	80 times ranked	10712 citing authors

#	Article	IF	Citations
1	Centering, scaling, and transformations: improving the biological information content of metabolomics data. BMC Genomics, 2006, 7, 142.	1.2	1,836
2	Assessment of PLSDA cross validation. Metabolomics, 2008, 4, 81-89.	1.4	1,178
3	Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies. Metabolomics, 2012, 8, 3-16.	1.4	622
4	Metabolic fate of polyphenols in the human superorganism. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4531-4538.	3.3	448
5	Reflections on univariate and multivariate analysis of metabolomics data. Metabolomics, 2014, 10, 361-374.	1.4	406
6	Multivariate paired data analysis: multilevel PLSDA versus OPLSDA. Metabolomics, 2010, 6, 119-128.	1.4	362
7	ASCA: analysis of multivariate data obtained from an experimental design. Journal of Chemometrics, 2005, 19, 469-481.	0.7	201
8	A framework for sequential multiblock component methods. Journal of Chemometrics, 2003, 17, 323-337.	0.7	190
9	Data-processing strategies for metabolomics studies. TrAC - Trends in Analytical Chemistry, 2011, 30, 1685-1698.	5.8	164
10	Multilevel Data Analysis of a Crossover Designed Human Nutritional Intervention Study. Journal of Proteome Research, 2008, 7, 4483-4491.	1.8	158
11	Statistical validation of megavariate effects in ASCA. BMC Bioinformatics, 2007, 8, 322.	1.2	137
12	Variable selection and validation in multivariate modelling. Bioinformatics, 2019, 35, 972-980.	1.8	122
13	ANOVAâ€“principal component analysis and ANOVAâ€“simultaneous component analysis: a comparison. Journal of Chemometrics, 2011, 25, 561-567.	0.7	119
14	Multiway multiblock component and covariates regression models. Journal of Chemometrics, 2000, 14, 301-331.	0.7	92
15	Phenotyping Tea Consumers by Nutrikinetic Analysis of Polyphenolic End-Metabolites. Journal of Proteome Research, 2009, 8, 3317-3330.	1.8	89
16	Deflation in multiblock PLS. Journal of Chemometrics, 2001, 15, 485-493.	0.7	81
17	Discriminant Q2 (DQ2) for improved discrimination in PLSDA models. Metabolomics, 2008, 4, 293-296.	1.4	69
18	Identifying inhibitory compounds in lignocellulosic biomass hydrolysates using an exometabolomics approach. BMC Biotechnology, 2014, 14, 22.	1.7	55

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19	Monitoring of batch processes using spectroscopy. AIChE Journal, 2002, 48, 2283-2297.	1.8	53
20	PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data. Journal of Chemometrics, 2008, 22, 114-121.	0.7	52
21	Harmonization of quality metrics and power calculation in multi-omic studies. Nature Communications, 2020, 11, 3092.	5.8	43
22	Variable importance in latent variable regression models. Journal of Chemometrics, 2014, 28, 615-622.	0.7	42
23	Modelling of spectroscopic batch process data using grey models to incorporate external information. Journal of Chemometrics, 2001, 15, 101-121.	0.7	38
24	StandardizedQ-statistic for improved sensitivity in the monitoring of residuals in MSPC. Journal of Chemometrics, 2000, 14, 335-349.	0.7	34
25	Lipidomic Response to Coffee Consumption. Nutrients, 2018, 10, 1851.	1.7	32
26	Effect of strigolactones on recruitment of the rice root-associated microbiome. FEMS Microbiology Ecology, 2022, 98, .	1.3	29
27	Metabolomics data exploration guided by prior knowledge. Analytica Chimica Acta, 2009, 651, 173-181.	2.6	28
28	Exploring the analysis of structured metabolomics data. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 88-96.	1.8	27
29	STATegra, a comprehensive multi-omics dataset of B-cell differentiation in mouse. Scientific Data, 2019, 6, 256.	2.4	26
30	Multiâ€way analysis of flux distributions across multiple conditions. Journal of Chemometrics, 2009, 23, 406-420.	0.7	23
31	Use of prior knowledge for the analysis of high-throughput transcriptomics and metabolomics data. BMC Systems Biology, 2014, 8, S2.	3.0	23
32	Contribution towards a Metabolite Profile of the Detoxification of Benzoic Acid through Glycine Conjugation: An Intervention Study. PLoS ONE, 2016, 11, e0167309.	1.1	23
33	New Figures of Merit for Comprehensive Functional Genomics Data: The Metabolomics Case. Analytical Chemistry, 2011, 83, 3267-3274.	3.2	22
34	Selecting the number of factors in principal component analysis by permutation testingâ€"Numerical and practical aspects. Journal of Chemometrics, 2017, 31, e2937.	0.7	22
35	Principal component analysis of binary genomics data. Briefings in Bioinformatics, 2019, 20, 317-329.	3.2	21
36	Repeated measures ASCA+ for analysis of longitudinal intervention studies with multivariate outcome data. PLoS Computational Biology, 2021, 17, e1009585.	1.5	21

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37	Population-based nutrikinetic modeling of polyphenol exposure. Metabolomics, 2014, 10, 1059-1073.	1.4	20
38	Integration of omics data to unravel root microbiome recruitment. Current Opinion in Biotechnology, 2021, 70, 255-261.	3.3	20
39	Grey component analysis. Journal of Chemometrics, 2007, 21, 474-485.	0.7	19
40	The geometry of ASCA. Journal of Chemometrics, 2008, 22, 464-471.	0.7	19
41	iTOP: inferring the topology of omics data. Bioinformatics, 2018, 34, i988-i996.	1.8	19
42	Near-Infrared Spectroscopic Monitoring of a Series of Industrial Batch Processes Using a Bilinear Grey Model. Applied Spectroscopy, 2003, 57, 1007-1019.	1.2	18
43	Separating common from distinctive variation. BMC Bioinformatics, 2016, 17, 195.	1.2	18
44	The 1H-NMR-based metabolite profile of acute alcohol consumption: A metabolomics intervention study. PLoS ONE, 2018, 13, e0196850.	1.1	18
45	Increased comparability between RNA-Seq and microarray data by utilization of gene sets. PLoS Computational Biology, 2020, 16, e1008295.	1.5	18
46	Tracyâ€“Widom statistic for the largest eigenvalue of autoscaled real matrices. Journal of Chemometrics, 2011, 25, 644-652.	0.7	17
47	Analyzing metabolomics-based challenge tests. Metabolomics, 2015, 11, 50-63.	1.4	17
48	Gut microbial activity as influenced by fiber digestion: dynamic metabolomics in an in vitro colon simulator. Metabolomics, 2016, 12, 1.	1.4	17
49	GCâ€“MS-based urinary organic acid profiling reveals multiple dysregulated metabolic pathways following experimental acute alcohol consumption. Scientific Reports, 2018, 8, 5775.	1.6	17
50	Simplivariate Models: Ideas and First Examples. PLoS ONE, 2008, 3, e3259.	1.1	16
51	Application of NMR-based metabonomics suggests a relationship between betaine absorption and elevated creatine plasma concentrations in catheterised sows. British Journal of Nutrition, 2012, 107, 1603-1615.	1.2	15
52	Model Selection and Optimal Sampling in High-Throughput Experimentation. Analytical Chemistry, 2004, 76, 3171-3178.	3.2	14
53	Performance assessment and improvement of control charts for statistical batch process monitoring. Statistica Neerlandica, 2006, 60, 339-360.	0.9	14
54	Simplivariate Models: Uncovering the Underlying Biology in Functional Genomics Data. PLoS ONE, 2011, 6, e20747.	1.1	13

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55	Common and distinct variation in data fusion of designed experimental data. Metabolomics, 2020, 16, 2.	1.4	13
56	Kinetic and mechanistic studies on the Heck reaction using real-time near infrared spectroscopy. Physical Chemistry Chemical Physics, 2003, 5, 4455-4460.	1.3	12
57	Weighted sparse principal component analysis. Chemometrics and Intelligent Laboratory Systems, 2019, 195, 103875.	1.8	10
58	Maximum likelihood scaling (MALS). Journal of Chemometrics, 2006, 20, 120-127.	0.7	9
59	Logistic principal component analysis via non-convex singular value thresholding. Chemometrics and Intelligent Laboratory Systems, 2020, 204, 104089.	1.8	9
60	Fusing metabolomics data sets with heterogeneous measurement errors. PLoS ONE, 2018, 13, e0195939.	1.1	7
61	Separating common (global and local) and distinct variation in multiple mixed types data sets. Journal of Chemometrics, 2020, 34, e3197.	0.7	7
62	Metabolomics variable selection and classification in the presence of observations below the detection limit using an extension of ERp. BMC Bioinformatics, 2017, 18, 83.	1.2	6
63	Elevation of fatty acid desaturaseÂ2 in esophageal adenocarcinoma increases polyunsaturated lipids and may exacerbate bile acidâ€induced DNA damage. Clinical and Translational Medicine, 2022, 12, e810.	1.7	6
64	Network Identification of Hormonal Regulation. PLoS ONE, 2014, 9, e96284.	1.1	5
65	Variable selection for binary classification using error rate p-values applied to metabolomics data. BMC Bioinformatics, 2016, 17, 33.	1.2	5
66	Training for translation between disciplines: a philosophy for life and data sciences curricula. Bioinformatics, 2018, 34, i4-i12.	1.8	5
67	Heterofusion: Fusing genomics data of different measurement scales. Journal of Chemometrics, 2021, 35, e3200.	0.7	5
68	A beginnerâ€™s guide to integrating multi-omics data from microbial communities. Biochemist, 2022, 44, 23-29.	0.2	5
69	Divide et impera: How disentangling common and distinctive variability in multiset data analysis can aid industrial process troubleshooting and understanding. Journal of Chemometrics, 2021, 35, e3266.	0.7	4
70	Generalized simultaneous component analysis of binary and quantitative data. Journal of Chemometrics, 2021, 35, e3312.	0.7	3
71	Systematic selection of competing metabolomics methods in a metabolite-sensory relationship study. Metabolomics, 2021, 17, 77.	1.4	3
72	Editorialâ€“data analysis in metabolomics. Metabolomics, 2012, 8, 1-2.	1.4	2

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73	A technical note on challenge tests in human volunteers for multidimensional phenotyping. Chemometrics and Intelligent Laboratory Systems, 2014, 136, 81-84.	1.8	2
74	Targeted proteomic response to coffee consumption. European Journal of Nutrition, 2020, 59, 1529-1539.	1.8	2
75	Topology of Transcriptional Regulatory Networks: Testing and Improving. PLoS ONE, 2012, 7, e40082.	1.1	1
76	Using Petri nets for experimental design in a multi-organ elimination pathway. Computers in Biology and Medicine, 2015, 63, 19-27.	3.9	1
77	Why orthogonal rotations might be not so orthogonal as you think. Journal of Chemometrics, 2017, 31, e2920.	0.7	1