Age K Smilde

List of Publications by Year
in descending order

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223 papers	19,079 citations	22099 59 h-index	13338 130 g-index
256 all docs	256 docs citations	256 times ranked	20024 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	Selectivity, local rank, three-way data analysis and ambiguity in multivariate curve resolution. Journal of Chemometrics, 1995, 9, 31-58.	0.7	868
4	Large-Scale Human Metabolomics Studies:â€‰ A Strategy for Data (Pre-) Processing and Validation. Analytical Chemistry, 2006, 78, 567-574.	3.2	744
5	Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies. Metabolomics, 2012, 8, 3-16.	1.4	622
6	ANOVA-simultaneous component analysis (ASCA): a new tool for analyzing designed metabolomics data. Bioinformatics, 2005, 21, 3043-3048.	1.8	552
7	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
8	Generalized contribution plots in multivariate statistical process monitoring. Chemometrics and Intelligent Laboratory Systems, 2000, 51, 95-114.	1.8	440
9	Reflections on univariate and multivariate analysis of metabolomics data. Metabolomics, 2014, 10, 361-374.	1.4	406
10	Multivariate paired data analysis: multilevel PLSDA versus OPLSDA. Metabolomics, 2010, 6, 119-128.	1.4	362
11	Proposed minimum reporting standards for data analysis in metabolomics. Metabolomics, 2007, 3, 231-241.	1.4	361
12	Centering and scaling in component analysis. Journal of Chemometrics, 2003, 17, 16-33.	0.7	327
13	Fusion of Mass Spectrometry-Based Metabolomics Data. Analytical Chemistry, 2005, 77, 6729-6736.	3.2	290
14	Atherosclerosis and liver inflammation induced by increased dietary cholesterol intake: a combined transcriptomics and metabolomics analysis. Genome Biology, 2007, 8, R200.	13.9	210
15	Influence of Temperature on Vibrational Spectra and Consequences for the Predictive Ability of Multivariate Models. Analytical Chemistry, 1998, 70, 1761-1767.	3.2	204
16	ASCA: analysis of multivariate data obtained from an experimental design. Journal of Chemometrics, 2005, 19, 469-481.	0.7	201
17	A framework for sequential multiblock component methods. Journal of Chemometrics, 2003, 17, 323-337.	0.7	190
18	Cellular and molecular synergy in AS01-adjuvanted vaccines results in an early IFNÎ³ response promoting vaccine immunogenicity. Npj Vaccines, 2017, 2, 25.	2.9	171

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19	Assessing the statistical validity of proteomics based biomarkers. Analytica Chimica Acta, 2007, 592, 210-217.	2.6	166
20	Data-processing strategies for metabolomics studies. TrAC - Trends in Analytical Chemistry, 2011, 30, 1685-1698.	5.8	164
21	Three-way analyses problems and prospects. Chemometrics and Intelligent Laboratory Systems, 1992, 15, 143-157.	1.8	161
22	Multilevel Data Analysis of a Crossover Designed Human Nutritional Intervention Study. Journal of Proteome Research, 2008, 7, 4483-4491.	1.8	158
23	Assessing the performance of statistical validation tools for megavariate metabolomics data. Metabolomics, 2006, 2, 53-61.	1.4	138
24	Statistical validation of megavariate effects in ASCA. BMC Bioinformatics, 2007, 8, 322.	1.2	137
25	A Critical Assessment of Feature Selection Methods for Biomarker Discovery in Clinical Proteomics. Molecular and Cellular Proteomics, 2013, 12, 263-276.	2.5	120
26	ANOVAâ€“principal component analysis and ANOVAâ€“simultaneous component analysis: a comparison. Journal of Chemometrics, 2011, 25, 561-567.	0.7	119
27	Symbiosis of chemometrics and metabolomics: past, present, and future. Journal of Chemometrics, 2005, 19, 376-386.	0.7	111
28	Critical evaluation of approaches for on-line batch process monitoring. Chemical Engineering Science, 2002, 57, 3979-3991.	1.9	110
29	Quantitative analysis of target components by comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2003, 1019, 15-29.	1.8	110
30	Metabolic Profiling of the Response to an Oral Glucose Tolerance Test Detects Subtle Metabolic Changes. PLoS ONE, 2009, 4, e4525.	1.1	105
31	Multilevel component analysis of time-resolved metabolic fingerprinting data. Analytica Chimica Acta, 2005, 530, 173-183.	2.6	96
32	Multiway multiblock component and covariates regression models. Journal of Chemometrics, 2000, 14, 301-331.	0.7	92
33	Correction of Temperature-Induced Spectral Variation by Continuous Piecewise Direct Standardization. Analytical Chemistry, 2000, 72, 1639-1644.	3.2	92
34	Data Fusion in Metabolomics Using Coupled Matrix and Tensor Factorizations. Proceedings of the IEEE, 2015, 103, 1602-1620.	16.4	92
35	A structured overview of simultaneous component based data integration. BMC Bioinformatics, 2009, 10, 246.	1.2	89
36	Phenotyping Tea Consumers by Nutrikinetic Analysis of Polyphenolic End-Metabolites. Journal of Proteome Research, 2009, 8, 3317-3330.	1.8	89

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37	Theory of medium-rank second-order calibration with restricted-Tucker models. Journal of Chemometrics, 1994, 8, 21-36.	0.7	87
38	Corruption of the Pearson correlation coefficient by measurement error and its estimation, bias, and correction under different error models. Scientific Reports, 2020, 10, 438.	1.6	87
39	Comments on multilinear PLS. Journal of Chemometrics, 1997, 11, 367-377.	0.7	85
40	Maximum likelihood fitting using ordinary least squares algorithms. Journal of Chemometrics, 2002, 16, 387-400.	0.7	85
41	Deflation in multiblock PLS. Journal of Chemometrics, 2001, 15, 485-493.	0.7	81
42	Discovering gene expression patterns in time course microarray experiments by ANOVAâ€“SCA. Bioinformatics, 2007, 23, 1792-1800.	1.8	80
43	A comparison of multiway regression and scaling methods. Chemometrics and Intelligent Laboratory Systems, 2001, 59, 121-136.	1.8	79
44	Optimized Time Alignment Algorithm for LCâ^'MS Data: Correlation Optimized Warping Using Component Detection Algorithm-Selected Mass Chromatograms. Analytical Chemistry, 2008, 80, 7012-7021.	3.2	79
45	Linear techniques to correct for temperature-induced spectral variation in multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2000, 51, 189-200.	1.8	78
46	The Muscle Metabolome Differs between Healthy and Frail Older Adults. Journal of Proteome Research, 2016, 15, 499-509.	1.8	76
47	Three-way methods for the calibration of chromatographic systems: Comparing PARAFAC and three-way PLS. Journal of Chemometrics, 1991, 5, 345-360.	0.7	75
48	Dynamic time warping of spectroscopic BATCH data. Analytica Chimica Acta, 2003, 498, 133-153.	2.6	74
49	Analysis of longitudinal metabolomics data. Bioinformatics, 2004, 20, 2438-2446.	1.8	74
50	Common and distinct components in data fusion. Journal of Chemometrics, 2017, 31, e2900.	0.7	71
51	A comparison of various methods for multivariate regression with highly collinear variables. Statistical Methods and Applications, 2007, 16, 193-228.	0.7	70
52	Calibration methods for complex second-order data. Analytica Chimica Acta, 1999, 398, 237-251.	2.6	69
53	Discriminant Q2 (DQ2) for improved discrimination in PLSDA models. Metabolomics, 2008, 4, 293-296.	1.4	69
54	Estimating rate constants and pure UV-vis spectra of a two-step reaction using trilinear models. Journal of Chemometrics, 1999, 13, 311-329.	0.7	67

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55	Estimating confidence intervals for principal component loadings: A comparison between the bootstrap and asymptotic results. British Journal of Mathematical and Statistical Psychology, 2007, 60, 295-314.	1.0	67
56	Gender-Dependent Associations of Metabolite Profiles and Body Fat Distribution in a Healthy Population with Central Obesity: Towards Metabolomics Diagnostics. OMICS A Journal of Integrative Biology, 2012, 16, 652-667.	1.0	61
57	Fault detection properties of global, local and time evolving models for batch process monitoring. Journal of Process Control, 2005, 15, 799-805.	1.7	60
58	Statistical data processing in clinical proteomics. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 866, 77-88.	1.2	60
59	Biomarkers for lysosomal storage disorders: identification and application as exemplified by chitotriosidase in Gaucher disease. Acta Paediatrica, International Journal of Paediatrics, 2008, 97, 7-14.	0.7	60
60	Multiway calibration in 3D QSAR. Journal of Chemometrics, 1997, 11, 511-524.	0.7	59
61	On the increase of predictive performance with high-level data fusion. Analytica Chimica Acta, 2011, 705, 41-47.	2.6	59
62	Cross-validation of multiway component models. Journal of Chemometrics, 1999, 13, 491-510.	0.7	56
63	On the difference between low-rank and subspace approximation: improved model for multi-linear PLS regression. Chemometrics and Intelligent Laboratory Systems, 2001, 58, 3-13.	1.8	56
64	Identifying inhibitory compounds in lignocellulosic biomass hydrolysates using an exometabolomics approach. BMC Biotechnology, 2014, 14, 22.	1.7	55
65	Monitoring and diagnosing batch processes with multiway covariates regression models. AICHE Journal, 1999, 45, 1504-1520.	1.8	53
66	Monitoring of batch processes using spectroscopy. AICHE Journal, 2002, 48, 2283-2297.	1.8	53
67	A generic linked-mode decomposition model for data fusion. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 83-94.	1.8	53
68	PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data. Journal of Chemometrics, 2008, 22, 114-121.	0.7	52
69	Time Alignment Algorithms Based on Selected Mass Traces for Complex LC-MS Data. Journal of Proteome Research, 2010, 9, 1483-1495.	1.8	52
70	Quantification of lipoprotein profiles by nuclear magnetic resonance spectroscopy and multivariate data analysis. TrAC - Trends in Analytical Chemistry, 2017, 94, 210-219.	5.8	52
71	Constrained three-mode factor analysis as a tool for parameter estimation with second-order instrumental data. Journal of Chemometrics, 1998, 12, 125-147.	0.7	51
72	Application of curve resolution based methods to kinetic data. Analytica Chimica Acta, 1999, 396, 231-240.	2.6	51

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73	Estimating reaction rate constants from a two-step reaction: a comparison between two-way and three-way methods. Journal of Chemometrics, 2000, 14, 541-560.	0.7	49
74	How to distinguish healthy from diseased? Classification strategy for mass spectrometryâ€based clinical proteomics. Proteomics, 2007, 7, 3672-3680.	1.3	49
75	Metabolic network discovery through reverse engineering of metabolome data. Metabolomics, 2009, 5, 318-329.	1.4	49
76	Some theoretical results on second-order calibration methods for data with and without rank overlap. Journal of Chemometrics, 1995, 9, 179-195.	0.7	48
77	Toward Reliable Lipoprotein Particle Predictions from NMR Spectra of Human Blood: An Interlaboratory Ring Test. Analytical Chemistry, 2017, 89, 8004-8012.	3.2	46
78	Comments on three-way analyses used for batch process data. Journal of Chemometrics, 2001, 15, 19-27.	0.7	44
79	Estimating reaction rate constants: comparison between traditional curve fitting and curve resolution. Analytica Chimica Acta, 2000, 419, 197-207.	2.6	42
80	Variable importance in latent variable regression models. Journal of Chemometrics, 2014, 28, 615-622.	0.7	42
81	Rapid estimation of rate constants using on-line SW-NIR and trilinear models. Analytica Chimica Acta, 1998, 376, 339-355.	2.6	41
82	A lipidomic analysis approach to evaluate the response to cholesterol-lowering food intake. Metabolomics, 2012, 8, 894-906.	1.4	40
83	Between Metabolite Relationships: an essential aspect of metabolic change. Metabolomics, 2012, 8, 422-432.	1.4	40
84	Revealing hidden information in GCâ€“MS spectra from isomeric drugs: Chemometrics based identification from 15ÂeV and 70ÂeV EI mass spectra. Forensic Chemistry, 2020, 18, 100225.	1.7	40
85	Applications and new developments of the direct exponential curve resolution algorithm (DECRA). Examples of spectra and magnetic resonance images. Journal of Chemometrics, 1999, 13, 95-110.	0.7	39
86	Monitoring a PVC Batch Process with Multivariate Statistical Process Control Charts. Industrial & Engineering Chemistry Research, 1999, 38, 4769-4776.	1.8	39
87	A Systematic Approach to Obtain Validated Partial Least Square Models for Predicting Lipoprotein Subclasses from Serum NMR Spectra. Analytical Chemistry, 2014, 86, 543-550.	3.2	39
88	Modelling of spectroscopic batch process data using grey models to incorporate external information. Journal of Chemometrics, 2001, 15, 101-121.	0.7	38
89	Rapid estimation of rate constants of batch processes using on-line SW-NIR. AICHE Journal, 1998, 44, 2713-2723.	1.8	36
90	DISCO-SCA and Properly Applied GSVD as Swinging Methods to Find Common and Distinctive Processes. PLoS ONE, 2012, 7, e37840.	1.1	36

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91	MetDFBA: incorporating time-resolved metabolomics measurements into dynamic flux balance analysis. Molecular BioSystems, 2015, 11, 137-145.	2.9	36
92	Multiway covariates regression models. Journal of Chemometrics, 1999, 13, 31-48.	0.7	35
93	The effect of the size of the training set and number of principal components on the false alarm rate in statistical process monitoring. Chemometrics and Intelligent Laboratory Systems, 2004, 73, 181-187.	1.8	35
94	GRID/GOLPE 3D Quantitative Structureâ^'Activity Relationship Study on a Set of Benzamides and Naphthamides, with Affinity for the Dopamine D3Receptor Subtype. Journal of Medicinal Chemistry, 1997, 40, 833-840.	2.9	34
95	StandardizedQ-statistic for improved sensitivity in the monitoring of residuals in MSPC. Journal of Chemometrics, 2000, 14, 335-349.	0.7	34
96	Insight in modulation of inflammation in response to diclofenac intervention: a human intervention study. BMC Medical Genomics, 2010, 3, 5.	0.7	34
97	Determination of Rate Constants in Second-Order Kinetics Using UV-Visible Spectroscopy. Applied Spectroscopy, 2001, 55, 77-83.	1.2	33
98	Scaling in ANOVA-simultaneous component analysis. Metabolomics, 2015, 11, 1265-1276.	1.4	33
99	Transcriptional profiles of adjuvanted hepatitis B vaccines display variable interindividual homogeneity but a shared core signature. Science Translational Medicine, 2020, 12, .	5.8	33
100	Spectroscopic Monitoring of Batch Reactions for On-Line Fault Detection and Diagnosis. Analytical Chemistry, 2000, 72, 5322-5330.	3.2	31
101	Improving the analysis of designed studies by combining statistical modelling with study design information. BMC Bioinformatics, 2009, 10, 52.	1.2	31
102	Gaucher disease: a model disorder for biomarker discovery. Expert Review of Proteomics, 2009, 6, 411-419.	1.3	31
103	Acute Effects of Morning Light on Plasma Glucose and Triglycerides in Healthy Men and Men with Type 2 Diabetes. Journal of Biological Rhythms, 2017, 32, 130-142.	1.4	30
104	Non-triviality and identification of a constrained Tucker3 analysis. Journal of Chemometrics, 2002, 16, 609-612.	0.7	29
105	Global test for metabolic pathway differences between conditions. Analytica Chimica Acta, 2012, 719, 8-15.	2.6	29
106	Effect of strigolactones on recruitment of the rice root-associated microbiome. FEMS Microbiology Ecology, 2022, 98, .	1.3	29
107	Calibration and detailed analysis of second-order flow injection analysis data with rank overlap. Analytica Chimica Acta, 2000, 422, 21-36.	2.6	28
108	Sufficient conditions for unique solutions within a certain class of curve resolution models. Journal of Chemometrics, 2001, 15, 405-411.	0.7	28

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109	Metabolomics data exploration guided by prior knowledge. Analytica Chimica Acta, 2009, 651, 173-181.	2.6	28
110	The photographer and the greenhouse: how to analyse plant metabolomics data. Phytochemical Analysis, 2010, 21, 48-60.	1.2	28
111	Exploring the analysis of structured metabolomics data. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 88-96.	1.8	27
112	Weight loss predictability by plasma metabolic signatures in adults with obesity and morbid obesity of the <scp>D</scp>i<scp>O</scp><scp>G</scp>enes study. Obesity, 2016, 24, 379-388.	1.5	27
113	Direct sampling tandem mass spectrometry (MS/MS) and multiway calibration for isomer quantitation. Analyst, The, 2002, 127, 1054-1060.	1.7	26
114	Analyzing Longitudinal Microbial Metabolomics Data. Journal of Proteome Research, 2009, 8, 4319-4327.	1.8	26
115	Online Detection and Identification Interferents in Multivariate Predictions of Organic Gases Using FT-IR Spectroscopy. Analytical Chemistry, 1995, 67, 2170-2179.	3.2	25
116	Reverse engineering of metabolic networks, a critical assessment. Molecular BioSystems, 2011, 7, 511-520.	2.9	24
117	A multiway 3D QSAR analysis of a series of (S)-N-[(1-ethyl-2-pyrrolidinyl)methyl]-6-methoxybenzamides. Journal of Computer-Aided Molecular Design, 1998, 12, 81-93.	1.3	23
118	Constrained least squares methods for estimating reaction rate constants from spectroscopic data. Journal of Chemometrics, 2002, 16, 28-40.	0.7	23
119	Multiâ€way analysis of flux distributions across multiple conditions. Journal of Chemometrics, 2009, 23, 406-420.	0.7	23
120	Use of prior knowledge for the analysis of high-throughput transcriptomics and metabolomics data. BMC Systems Biology, 2014, 8, S2.	3.0	23
121	Bootstrap confidence intervals in multiâ€level simultaneous component analysis. British Journal of Mathematical and Statistical Psychology, 2009, 62, 299-318.	1.0	22
122	New Figures of Merit for Comprehensive Functional Genomics Data: The Metabolomics Case. Analytical Chemistry, 2011, 83, 3267-3274.	3.2	22
123	Of Monkeys and Men: A Metabolomic Analysis of Static and Dynamic Urinary Metabolic Phenotypes in Two Species. PLoS ONE, 2014, 9, e106077.	1.1	22
124	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
125	Generic framework for high-dimensional fixed-effects ANOVA. Briefings in Bioinformatics, 2012, 13, 524-535.	3.2	21
126	Principal component analysis of binary genomics data. Briefings in Bioinformatics, 2019, 20, 317-329.	3.2	21

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127	Repeated measures ASCA+ for analysis of longitudinal intervention studies with multivariate outcome data. PLoS Computational Biology, 2021, 17, e1009585.	1.5	21
128	Multivariate calibration of reversed-phase chromatographic systems. Some designs based on three-way data analysis. Analytica Chimica Acta, 1990, 235, 41-51.	2.6	20
129	Population-based nutrikinetic modeling of polyphenol exposure. Metabolomics, 2014, 10, 1059-1073.	1.4	20
130	Validation and selection of ODE based systems biology models: how to arrive at more reliable decisions. BMC Systems Biology, 2015, 9, 32.	3.0	20
131	Confidence ellipsoids for ASCA models based on multivariate regression theory. Journal of Chemometrics, 2018, 32, e2990.	0.7	20
132	Integration of omics data to unravel root microbiome recruitment. Current Opinion in Biotechnology, 2021, 70, 255-261.	3.3	20
133	Grey component analysis. Journal of Chemometrics, 2007, 21, 474-485.	0.7	19
134	The geometry of ASCA. Journal of Chemometrics, 2008, 22, 464-471.	0.7	19
135	A Classification Model for the Leiden Proteomics Competition. Statistical Applications in Genetics and Molecular Biology, 2008, 7, Article8.	0.2	19
136	Characterizing the precision of mass-spectrometry-based metabolic profiling platforms. Analyst, The, 2009, 134, 2281.	1.7	19
137	iTOP: inferring the topology of omics data. Bioinformatics, 2018, 34, i988-i996.	1.8	19
138	Optimizing Meta-Parameters in Continuous Piecewise Direct Standardization. Applied Spectroscopy, 2001, 55, 458-466.	1.2	18
139	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
140	Performance Optimization of Spectroscopic Process Analyzers. Analytical Chemistry, 2004, 76, 2656-2663.	3.2	18
141	Identification of prognostic and diagnostic biomarkers of glucose intolerance in ApoE3Leiden mice. Physiological Genomics, 2012, 44, 293-304.	1.0	18
142	Separating common from distinctive variation. BMC Bioinformatics, 2016, 17, 195.	1.2	18
143	Group-wise ANOVA simultaneous component analysis for designed omics experiments. Metabolomics, 2018, 14, 73.	1.4	18
144	Increased comparability between RNA-Seq and microarray data by utilization of gene sets. PLoS Computational Biology, 2020, 16, e1008295.	1.5	18

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145	Simple validatory tools for judging the predictive performance of parafac and three-way PLS. Journal of Chemometrics, 1992, 6, 11-28.	0.7	17
146	Selection of Optimal Process Analyzers for Plant-Wide Monitoring. Analytical Chemistry, 2002, 74, 3105-3111.	3.2	17
147	Tracyâ€“Widom statistic for the largest eigenvalue of autoscaled real matrices. Journal of Chemometrics, 2011, 25, 644-652.	0.7	17
148	Analyzing metabolomics-based challenge tests. Metabolomics, 2015, 11, 50-63.	1.4	17
149	Simplivariate Models: Ideas and First Examples. PLoS ONE, 2008, 3, e3259.	1.1	16
150	Individual differences in metabolomics: individualised responses and between-metabolite relationships. Metabolomics, 2012, 8, 94-104.	1.4	16
151	Performance of methods that separate common and distinct variation in multiple data blocks. Journal of Chemometrics, 2019, 33, e3085.	0.7	16
152	Assessing the metabolic effects of prednisolone in healthy volunteers using urine metabolic profiling. Genome Medicine, 2012, 4, 94.	3.6	15
153	Covariances Simultaneous Component Analysis: a new method within a framework for modeling covariances. Journal of Chemometrics, 2015, 29, 277-288.	0.7	15
154	Normalization techniques for PARAFAC modeling of urine metabolomic data. Metabolomics, 2016, 12, 1.	1.4	15
155	Performance assessment and improvement of control charts for statistical batch process monitoring. Statistica Neerlandica, 2006, 60, 339-360.	0.9	14
156	Crossfit analysis: a novel method to characterize the dynamics of induced plant responses. BMC Bioinformatics, 2009, 10, 425.	1.2	14
157	Nutrikinetic modeling reveals order of genistein phase II metabolites appearance in human plasma. Molecular Nutrition and Food Research, 2014, 58, 2111-2121.	1.5	14
158	An introduction to Multi-block Component Analysis by means of a flavor language case study. Food Quality and Preference, 2003, 14, 497-506.	2.3	13
159	Integrating functional genomics data using maximum likelihood based simultaneous component analysis. BMC Bioinformatics, 2009, 10, 340.	1.2	13
160	Endocrine pulse identification using penalized methods and a minimum set of assumptions. American Journal of Physiology - Endocrinology and Metabolism, 2010, 298, E146-E155.	1.8	13
161	Simplivariate Models: Uncovering the Underlying Biology in Functional Genomics Data. PLoS ONE, 2011, 6, e20747.	1.1	13
162	Common and distinct variation in data fusion of designed experimental data. Metabolomics, 2020, 16, 2.	1.4	13

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163	Choosing proper normalization is essential for discovery of sparse glycan biomarkers. Molecular Omics, 2020, 16, 231-242.	1.4	13
164	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
165	Tutorial: Correction of shifts in single-stage LC-MS(/MS) data. Analytica Chimica Acta, 2018, 999, 37-53.	2.6	12
166	A comparison of two <scp>PLS</scp>â€based approaches to structural equation modeling. Journal of Chemometrics, 2019, 33, e3105.	0.7	11
167	Identification of Analytical Factors Affecting Complex Proteomics Profiles Acquired in a Factorial Design Study with Analysis of Variance: Simultaneous Component Analysis. Analytical Chemistry, 2016, 88, 4229-4238.	3.2	10
168	Data representations and -analyses of binary diary data in pursuit of stratifying children based on common childhood illnesses. PLoS ONE, 2018, 13, e0207177.	1.1	10
169	Weighted sparse principal component analysis. Chemometrics and Intelligent Laboratory Systems, 2019, 195, 103875.	1.8	10
170	Characterization of stationary/mobile phase combinations by using markers. Analytica Chimica Acta, 1988, 212, 95-104.	2.6	9
171	Fast On-Line Analysis of Process Alkane Gas Mixtures by NIR Spectroscopy. Applied Spectroscopy, 2000, 54, 406-412.	1.2	9
172	Maximum likelihood scaling (MALS). Journal of Chemometrics, 2006, 20, 120-127.	0.7	9
173	To aggregate or not to aggregate high-dimensional classifiers. BMC Bioinformatics, 2011, 12, 153.	1.2	9
174	Logistic principal component analysis via non-convex singular value thresholding. Chemometrics and Intelligent Laboratory Systems, 2020, 204, 104089.	1.8	9
175	Sequential and orthogonalized PLS (SOâ€PLS) regression for path analysis: Order of blocks and relations between effects. Journal of Chemometrics, 2021, 35, e3243.	0.7	9
176	Human Blood Lipoprotein Predictions from ¹H NMR Spectra: Protocol, Model Performances, and Cage of Covariance. Analytical Chemistry, 2022, 94, 628-636.	3.2	9
177	Peer Reviewed: How to Choose the Right Process Analyzer. Analytical Chemistry, 2002, 74, 368 A-373 A.	3.2	8
178	Tackling Calibration Problems of Spectroscopic Analysis in High-Throughput Experimentation. Analytical Chemistry, 2005, 77, 2227-2234.	3.2	8
179	Profiling of Liquid Crystal Displays with Raman Spectroscopy: Preprocessing of Spectra. Applied Spectroscopy, 2005, 59, 267-274.	1.2	8
180	Manufacturing Vaccines: An Illustration of Using PAT Tools for Controlling the Cultivation ofBordetella pertussis. Quality Engineering, 2007, 19, 373-384.	0.7	8

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181	Comparability problems in the analysis of multiway data. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 2-11.	1.8	8
182	A Framework for Low-Level Data Fusion. Data Handling in Science and Technology, 2019, , 27-50.	3.1	8
183	Estimating kinetic parameters of complex catalytic reactions using a curve resolution based method. Chemometrics and Intelligent Laboratory Systems, 2008, 91, 101-109.	1.8	7
184	Correlated measurement error hampers association network inference. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2014, 966, 93-99.	1.2	7
185	Fusing metabolomics data sets with heterogeneous measurement errors. PLoS ONE, 2018, 13, e0195939.	1.1	7
186	Dynamic elementary mode modelling of non-steady state flux data. BMC Systems Biology, 2018, 12, 71.	3.0	7
187	Separating common (global and local) and distinct variation in multiple mixed types data sets. Journal of Chemometrics, 2020, 34, e3197.	0.7	7
188	Unraveling VEALYL Amyloid Formation Using Advanced Vibrational Spectroscopy and Microscopy. Biophysical Journal, 2020, 119, 87-98.	0.2	7
189	Multivariate quality assessment of aged RP-HPLC columns. Journal of Chemometrics, 1996, 10, 351-370.	0.7	6
190	Variable Selection Methods as a Tool To Find Sensor Locations for Distributed Parameter Systems. Industrial & Engineering Chemistry Research, 2008, 47, 1184-1191.	1.8	6
191	Discovery of subtle effects in a human intervention trial through multilevel modeling. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 108-114.	1.8	6
192	Strategies for Individual Phenotyping of Linoleic and Arachidonic Acid Metabolism Using an Oral Glucose Tolerance Test. PLoS ONE, 2015, 10, e0119856.	1.1	6
193	Repeatability and reproducibility of lipoprotein particle profile measurements in plasma samples by ultracentrifugation. Clinical Chemistry and Laboratory Medicine, 2019, 58, 103-115.	1.4	6
194	Process analyzer location and performance assessment for optimal process monitoring. AICHE Journal, 2001, 47, 2503-2514.	1.8	5
195	Detecting Regulatory Mechanisms in Endocrine Time Series Measurements. PLoS ONE, 2012, 7, e32985.	1.1	5
196	Inferring proteinâ€“protein interaction complexes from immunoprecipitation data. BMC Research Notes, 2013, 6, 468.	0.6	5
197	Network Identification of Hormonal Regulation. PLoS ONE, 2014, 9, e96284.	1.1	5
198	How informative is your kinetic model?: using resampling methods for model invalidation. BMC Systems Biology, 2014, 8, 61.	3.0	5

#	Article	IF	Citations
199	Heterofusion: Fusing genomics data of different measurement scales. Journal of Chemometrics, 2021, 35, e3200.	0.7	5
200	Exploring dynamic metabolomics data with multiway data analysis: a simulation study. BMC Bioinformatics, 2022, 23, 31.	1.2	5
201	Reply to ?Comment on a recently proposed resampling method?. Journal of Chemometrics, 2001, 15, 189-192.	0.7	4
202	Linking PCA and time derivatives of dynamic systems. Journal of Chemometrics, 2006, 20, 43-53.	0.7	4
203	Inversion of peak elution order prevents uniform time alignment of complex liquid-chromatography coupled to mass spectrometry datasets. Journal of Chromatography A, 2014, 1373, 61-72.	1.8	4
204	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
205	Chapter 12 Multivariate characterization of RP-HPLC stationary phases. Journal of Chromatography Library, 1995, 57, 403-449.	0.1	3
206	Single channel event (SCE) for managing sensor failures in MSPC. Computers and Chemical Engineering, 2006, 30, 961-969.	2.0	3
207	Generalized simultaneous component analysis of binary and quantitative data. Journal of Chemometrics, 2021, 35, e3312.	0.7	3
208	Systematic selection of competing metabolomics methods in a metabolite-sensory relationship study. Metabolomics, 2021, 17, 77.	1.4	3
209	A Theoretical Framework for Real Time Release with NIR and Chemometrics. NIR News, 2006, 17, 4-6.	1.6	2
210	Identification and quantification of sources of variation in the analysis of steel. Fresenius' Journal of Analytical Chemistry, 2000, 368, 397-406.	1.5	1
211	Computational modeling of the human serum proteome response to colon resection surgery. Analytica Chimica Acta, 2010, 661, 20-27.	2.6	1
212	Topology of Transcriptional Regulatory Networks: Testing and Improving. PLoS ONE, 2012, 7, e40082.	1.1	1
213	Not Just a Sum? Identifying Different Types of Interplay between Constituents in Combined Interventions. PLoS ONE, 2015, 10, e0125334.	1.1	1
214	Using Petri nets for experimental design in a multi-organ elimination pathway. Computers in Biology and Medicine, 2015, 63, 19-27.	3.9	1
215	Numerical Representations of Metabolic Systems. Analytical Chemistry, 2020, 92, 13614-13621.	3.2	1
216	Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements. Analytica Chimica Acta, 2021, 1185, 339073.	2.6	1

#	Article	IF	Citations
217	A Systematic Quantification of the Sources of Variation of Process Analytical Measurements in the Steel Industry. Quality Engineering, 2003, 15, 391-402.	0.7	0
218	Optimal measurement design for monitoring batch processes. AICHE Journal, 2010, 56, 837-840.	1.8	0
219	Report of the meeting TRICAP 2009, ThRee-way methods In Chemistry And Psychology. Chemometrics and Intelligent Laboratory Systems, 2009, 99, 161.	1.8	0
220	Inferring differences in the distribution of reaction rates across conditions. Molecular BioSystems, 2012, 8, 2415.	2.9	0
221	Towards a Hierarchical Strategy to Explore Multi-Scale IP/MS Data for Protein Complexes. PLoS ONE, 2015, 10, e0139704.	1.1	0
222	TRICAP 2018 Angel Fire Resort, New Mexico. Journal of Chemometrics, 2021, 35, e3313.	0.7	0
223	On using kernel integration by graphical LASSO to study partial correlations between heterogeneous data sets. Journal of Chemometrics, 2021, 35, e3324.	0.7	0