

Age K Smilde

List of Publications by Year in descending order

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223
papers

19,079
citations

22099

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h-index

13338

130
g-index

256
all docs

256
docs citations

256
times ranked

20024
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring dynamic metabolomics data with multiway data analysis: a simulation study. BMC Bioinformatics, 2022, 23, 31.	1.2	5
2	Effect of strigolactones on recruitment of the rice root-associated microbiome. FEMS Microbiology Ecology, 2022, 98, .	1.3	29
3	Human Blood Lipoprotein Predictions from ¹ H NMR Spectra: Protocol, Model Performances, and Cage of Covariance. Analytical Chemistry, 2022, 94, 628-636.	3.2	9
4	Sequential and orthogonalized PLS (SO-PLS) regression for path analysis: Order of blocks and relations between effects. Journal of Chemometrics, 2021, 35, e3243.	0.7	9
5	Heterofusion: Fusing genomics data of different measurement scales. Journal of Chemometrics, 2021, 35, e3200.	0.7	5
6	<i>Divide et impera</i> : 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
7	Generalized simultaneous component analysis of binary and quantitative data. Journal of Chemometrics, 2021, 35, e3312.	0.7	3
8	TRICAP 2018 Angel Fire Resort, New Mexico. Journal of Chemometrics, 2021, 35, e3313.	0.7	0
9	Systematic selection of competing metabolomics methods in a metabolite-sensory relationship study. Metabolomics, 2021, 17, 77.	1.4	3
10	Integration of omics data to unravel root microbiome recruitment. Current Opinion in Biotechnology, 2021, 70, 255-261.	3.3	20
11	Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements. Analytica Chimica Acta, 2021, 1185, 339073.	2.6	1
12	On using kernel integration by graphical LASSO to study partial correlations between heterogeneous data sets. Journal of Chemometrics, 2021, 35, e3324.	0.7	0
13	Repeated measures ASCA+ for analysis of longitudinal intervention studies with multivariate outcome data. PLoS Computational Biology, 2021, 17, e1009585.	1.5	21
14	Common and distinct variation in data fusion of designed experimental data. Metabolomics, 2020, 16, 2.	1.4	13
15	Separating common (global and local) and distinct variation in multiple mixed types data sets. Journal of Chemometrics, 2020, 34, e3197.	0.7	7
16	Increased comparability between RNA-Seq and microarray data by utilization of gene sets. PLoS Computational Biology, 2020, 16, e1008295.	1.5	18
17	Numerical Representations of Metabolic Systems. Analytical Chemistry, 2020, 92, 13614-13621.	3.2	1
18	Logistic principal component analysis via non-convex singular value thresholding. Chemometrics and Intelligent Laboratory Systems, 2020, 204, 104089.	1.8	9

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19	Transcriptional profiles of adjuvanted hepatitis B vaccines display variable interindividual homogeneity but a shared core signature. <i>Science Translational Medicine</i> , 2020, 12, .	5.8	33
20	Unraveling VEALYL Amyloid Formation Using Advanced Vibrational Spectroscopy and Microscopy. <i>Biophysical Journal</i> , 2020, 119, 87-98.	0.2	7
21	Choosing proper normalization is essential for discovery of sparse glycan biomarkers. <i>Molecular Omics</i> , 2020, 16, 231-242.	1.4	13
22	Corruption of the Pearson correlation coefficient by measurement error and its estimation, bias, and correction under different error models. <i>Scientific Reports</i> , 2020, 10, 438.	1.6	87
23	Revealing hidden information in GC-MS spectra from isomeric drugs: Chemometrics based identification from 15ÅeV and 70ÅeV EI mass spectra. <i>Forensic Chemistry</i> , 2020, 18, 100225.	1.7	40
24	Weighted sparse principal component analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 195, 103875.	1.8	10
25	A Framework for Low-Level Data Fusion. <i>Data Handling in Science and Technology</i> , 2019, , 27-50.	3.1	8
26	Repeatability and reproducibility of lipoprotein particle profile measurements in plasma samples by ultracentrifugation. <i>Clinical Chemistry and Laboratory Medicine</i> , 2019, 58, 103-115.	1.4	6
27	A comparison of two <scp>PLS</scp>-based approaches to structural equation modeling. <i>Journal of Chemometrics</i> , 2019, 33, e3105.	0.7	11
28	Performance of methods that separate common and distinct variation in multiple data blocks. <i>Journal of Chemometrics</i> , 2019, 33, e3085.	0.7	16
29	Principal component analysis of binary genomics data. <i>Briefings in Bioinformatics</i> , 2019, 20, 317-329.	3.2	21
30	Confidence ellipsoids for ASCA models based on multivariate regression theory. <i>Journal of Chemometrics</i> , 2018, 32, e2990.	0.7	20
31	Tutorial: Correction of shifts in single-stage LC-MS(/MS) data. <i>Analytica Chimica Acta</i> , 2018, 999, 37-53.	2.6	12
32	Data representations and -analyses of binary diary data in pursuit of stratifying children based on common childhood illnesses. <i>PLoS ONE</i> , 2018, 13, e0207177.	1.1	10
33	iTOP: inferring the topology of omics data. <i>Bioinformatics</i> , 2018, 34, i988-i996.	1.8	19
34	Fusing metabolomics data sets with heterogeneous measurement errors. <i>PLoS ONE</i> , 2018, 13, e0195939.	1.1	7
35	Dynamic elementary mode modelling of non-steady state flux data. <i>BMC Systems Biology</i> , 2018, 12, 71.	3.0	7
36	Group-wise ANOVA simultaneous component analysis for designed omics experiments. <i>Metabolomics</i> , 2018, 14, 73.	1.4	18

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37	Acute Effects of Morning Light on Plasma Glucose and Triglycerides in Healthy Men and Men with Type 2 Diabetes. <i>Journal of Biological Rhythms</i> , 2017, 32, 130-142.	1.4	30
38	Common and distinct components in data fusion. <i>Journal of Chemometrics</i> , 2017, 31, e2900.	0.7	71
39	Selecting the number of factors in principal component analysis by permutation testing—Numerical and practical aspects. <i>Journal of Chemometrics</i> , 2017, 31, e2937.	0.7	22
40	Cellular and molecular synergy in AS01-adjuvanted vaccines results in an early IFN γ response promoting vaccine immunogenicity. <i>Npj Vaccines</i> , 2017, 2, 25.	2.9	171
41	Quantification of lipoprotein profiles by nuclear magnetic resonance spectroscopy and multivariate data analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2017, 94, 210-219.	5.8	52
42	Toward Reliable Lipoprotein Particle Predictions from NMR Spectra of Human Blood: An Interlaboratory Ring Test. <i>Analytical Chemistry</i> , 2017, 89, 8004-8012.	3.2	46
43	Weight loss predictability by plasma metabolic signatures in adults with obesity and morbid obesity of the DIOGENES study. <i>Obesity</i> , 2016, 24, 379-388.	1.5	27
44	Separating common from distinctive variation. <i>BMC Bioinformatics</i> , 2016, 17, 195.	1.2	18
45	Normalization techniques for PARAFAC modeling of urine metabolomic data. <i>Metabolomics</i> , 2016, 12, 1.	1.4	15
46	Identification of Analytical Factors Affecting Complex Proteomics Profiles Acquired in a Factorial Design Study with Analysis of Variance: Simultaneous Component Analysis. <i>Analytical Chemistry</i> , 2016, 88, 4229-4238.	3.2	10
47	The Muscle Metabolome Differs between Healthy and Frail Older Adults. <i>Journal of Proteome Research</i> , 2016, 15, 499-509.	1.8	76
48	Covariances Simultaneous Component Analysis: a new method within a framework for modeling covariances. <i>Journal of Chemometrics</i> , 2015, 29, 277-288.	0.7	15
49	Strategies for Individual Phenotyping of Linoleic and Arachidonic Acid Metabolism Using an Oral Glucose Tolerance Test. <i>PLoS ONE</i> , 2015, 10, e0119856.	1.1	6
50	Not Just a Sum? Identifying Different Types of Interplay between Constituents in Combined Interventions. <i>PLoS ONE</i> , 2015, 10, e0125334.	1.1	1
51	Towards a Hierarchical Strategy to Explore Multi-Scale IP/MS Data for Protein Complexes. <i>PLoS ONE</i> , 2015, 10, e0139704.	1.1	0
52	MetDFBA: incorporating time-resolved metabolomics measurements into dynamic flux balance analysis. <i>Molecular BioSystems</i> , 2015, 11, 137-145.	2.9	36
53	Using Petri nets for experimental design in a multi-organ elimination pathway. <i>Computers in Biology and Medicine</i> , 2015, 63, 19-27.	3.9	1
54	Scaling in ANOVA-simultaneous component analysis. <i>Metabolomics</i> , 2015, 11, 1265-1276.	1.4	33

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55	Validation and selection of ODE based systems biology models: how to arrive at more reliable decisions. <i>BMC Systems Biology</i> , 2015, 9, 32.	3.0	20
56	Data Fusion in Metabolomics Using Coupled Matrix and Tensor Factorizations. <i>Proceedings of the IEEE</i> , 2015, 103, 1602-1620.	16.4	92
57	Analyzing metabolomics-based challenge tests. <i>Metabolomics</i> , 2015, 11, 50-63.	1.4	17
58	Network Identification of Hormonal Regulation. <i>PLoS ONE</i> , 2014, 9, e96284.	1.1	5
59	Of Monkeys and Men: A Metabolomic Analysis of Static and Dynamic Urinary Metabolic Phenotypes in Two Species. <i>PLoS ONE</i> , 2014, 9, e106077.	1.1	22
60	Inversion of peak elution order prevents uniform time alignment of complex liquid-chromatography coupled to mass spectrometry datasets. <i>Journal of Chromatography A</i> , 2014, 1373, 61-72.	1.8	4
61	Reflections on univariate and multivariate analysis of metabolomics data. <i>Metabolomics</i> , 2014, 10, 361-374.	1.4	406
62	Variable importance in latent variable regression models. <i>Journal of Chemometrics</i> , 2014, 28, 615-622.	0.7	42
63	A Systematic Approach to Obtain Validated Partial Least Square Models for Predicting Lipoprotein Subclasses from Serum NMR Spectra. <i>Analytical Chemistry</i> , 2014, 86, 543-550.	3.2	39
64	Population-based nutrkinetic modeling of polyphenol exposure. <i>Metabolomics</i> , 2014, 10, 1059-1073.	1.4	20
65	Identifying inhibitory compounds in lignocellulosic biomass hydrolysates using an exometabolomics approach. <i>BMC Biotechnology</i> , 2014, 14, 22.	1.7	55
66	How informative is your kinetic model?: using resampling methods for model invalidation. <i>BMC Systems Biology</i> , 2014, 8, 61.	3.0	5
67	Use of prior knowledge for the analysis of high-throughput transcriptomics and metabolomics data. <i>BMC Systems Biology</i> , 2014, 8, S2.	3.0	23
68	Correlated measurement error hampers association network inference. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2014, 966, 93-99.	1.2	7
69	Nutrkinetic modeling reveals order of genistein phase II metabolites appearance in human plasma. <i>Molecular Nutrition and Food Research</i> , 2014, 58, 2111-2121.	1.5	14
70	Inferring protein-protein interaction complexes from immunoprecipitation data. <i>BMC Research Notes</i> , 2013, 6, 468.	0.6	5
71	A Critical Assessment of Feature Selection Methods for Biomarker Discovery in Clinical Proteomics. <i>Molecular and Cellular Proteomics</i> , 2013, 12, 263-276.	2.5	120
72	Generic framework for high-dimensional fixed-effects ANOVA. <i>Briefings in Bioinformatics</i> , 2012, 13, 524-535.	3.2	21

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73	Identification of prognostic and diagnostic biomarkers of glucose intolerance in ApoE3Leiden mice. <i>Physiological Genomics</i> , 2012, 44, 293-304.	1.0	18
74	A lipidomic analysis approach to evaluate the response to cholesterol-lowering food intake. <i>Metabolomics</i> , 2012, 8, 894-906.	1.4	40
75	Inferring differences in the distribution of reaction rates across conditions. <i>Molecular BioSystems</i> , 2012, 8, 2415.	2.9	0
76	Gender-Dependent Associations of Metabolite Profiles and Body Fat Distribution in a Healthy Population with Central Obesity: Towards Metabolomics Diagnostics. <i>OMICS A Journal of Integrative Biology</i> , 2012, 16, 652-667.	1.0	61
77	Global test for metabolic pathway differences between conditions. <i>Analytica Chimica Acta</i> , 2012, 719, 8-15.	2.6	29
78	Assessing the metabolic effects of prednisolone in healthy volunteers using urine metabolic profiling. <i>Genome Medicine</i> , 2012, 4, 94.	3.6	15
79	Detecting Regulatory Mechanisms in Endocrine Time Series Measurements. <i>PLoS ONE</i> , 2012, 7, e32985.	1.1	5
80	DISCO-SCA and Properly Applied GSVD as Swinging Methods to Find Common and Distinctive Processes. <i>PLoS ONE</i> , 2012, 7, e37840.	1.1	36
81	Topology of Transcriptional Regulatory Networks: Testing and Improving. <i>PLoS ONE</i> , 2012, 7, e40082.	1.1	1
82	Individual differences in metabolomics: individualised responses and between-metabolite relationships. <i>Metabolomics</i> , 2012, 8, 94-104.	1.4	16
83	Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies. <i>Metabolomics</i> , 2012, 8, 3-16.	1.4	622
84	Between Metabolite Relationships: an essential aspect of metabolic change. <i>Metabolomics</i> , 2012, 8, 422-432.	1.4	40
85	Metabolic fate of polyphenols in the human superorganism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 4531-4538.	3.3	448
86	New Figures of Merit for Comprehensive Functional Genomics Data: The Metabolomics Case. <i>Analytical Chemistry</i> , 2011, 83, 3267-3274.	3.2	22
87	Reverse engineering of metabolic networks, a critical assessment. <i>Molecular BioSystems</i> , 2011, 7, 511-520.	2.9	24
88	On the increase of predictive performance with high-level data fusion. <i>Analytica Chimica Acta</i> , 2011, 705, 41-47.	2.6	59
89	Simplivariate Models: Uncovering the Underlying Biology in Functional Genomics Data. <i>PLoS ONE</i> , 2011, 6, e20747.	1.1	13
90	Data-processing strategies for metabolomics studies. <i>TrAC - Trends in Analytical Chemistry</i> , 2011, 30, 1685-1698.	5.8	164

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91	To aggregate or not to aggregate high-dimensional classifiers. BMC Bioinformatics, 2011, 12, 153.	1.2	9
92	ANOVAâ€“principal component analysis and ANOVAâ€“simultaneous component analysis: a comparison. Journal of Chemometrics, 2011, 25, 561-567.	0.7	119
93	Tracyâ€“Widom statistic for the largest eigenvalue of autoscaled real matrices. Journal of Chemometrics, 2011, 25, 644-652.	0.7	17
94	Discovery of subtle effects in a human intervention trial through multilevel modeling. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 108-114.	1.8	6
95	Comparability problems in the analysis of multiway data. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 2-11.	1.8	8
96	Optimal measurement design for monitoring batch processes. AIChE Journal, 2010, 56, 837-840.	1.8	0
97	Computational modeling of the human serum proteome response to colon resection surgery. Analytica Chimica Acta, 2010, 661, 20-27.	2.6	1
98	Multivariate paired data analysis: multilevel PLSDA versus OPLSDA. Metabolomics, 2010, 6, 119-128.	1.4	362
99	A generic linked-mode decomposition model for data fusion. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 83-94.	1.8	53
100	Insight in modulation of inflammation in response to diclofenac intervention: a human intervention study. BMC Medical Genomics, 2010, 3, 5.	0.7	34
101	The photographer and the greenhouse: how to analyse plant metabolomics data. Phytochemical Analysis, 2010, 21, 48-60.	1.2	28
102	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
103	Time Alignment Algorithms Based on Selected Mass Traces for Complex LC-MS Data. Journal of Proteome Research, 2010, 9, 1483-1495.	1.8	52
104	A structured overview of simultaneous component based data integration. BMC Bioinformatics, 2009, 10, 246.	1.2	89
105	Integrating functional genomics data using maximum likelihood based simultaneous component analysis. BMC Bioinformatics, 2009, 10, 340.	1.2	13
106	Crossfit analysis: a novel method to characterize the dynamics of induced plant responses. BMC Bioinformatics, 2009, 10, 425.	1.2	14
107	Improving the analysis of designed studies by combining statistical modelling with study design information. BMC Bioinformatics, 2009, 10, 52.	1.2	31
108	Multiâ€“way analysis of flux distributions across multiple conditions. Journal of Chemometrics, 2009, 23, 406-420.	0.7	23

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109	Metabolomics data exploration guided by prior knowledge. <i>Analytica Chimica Acta</i> , 2009, 651, 173-181.	2.6	28
110	Metabolic network discovery through reverse engineering of metabolome data. <i>Metabolomics</i> , 2009, 5, 318-329.	1.4	49
111	Exploring the analysis of structured metabolomics data. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2009, 98, 88-96.	1.8	27
112	Report of the meeting TRICAP 2009, ThRee-way methods In Chemistry And Psychology. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2009, 99, 161.	1.8	0
113	Bootstrap confidence intervals in multi-level simultaneous component analysis. <i>British Journal of Mathematical and Statistical Psychology</i> , 2009, 62, 299-318.	1.0	22
114	Phenotyping Tea Consumers by Nutrikinetic Analysis of Polyphenolic End-Metabolites. <i>Journal of Proteome Research</i> , 2009, 8, 3317-3330.	1.8	89
115	Analyzing Longitudinal Microbial Metabolomics Data. <i>Journal of Proteome Research</i> , 2009, 8, 4319-4327.	1.8	26
116	Characterizing the precision of mass-spectrometry-based metabolic profiling platforms. <i>Analyst, The</i> , 2009, 134, 2281.	1.7	19
117	Gaucher disease: a model disorder for biomarker discovery. <i>Expert Review of Proteomics</i> , 2009, 6, 411-419.	1.3	31
118	Metabolic Profiling of the Response to an Oral Glucose Tolerance Test Detects Subtle Metabolic Changes. <i>PLoS ONE</i> , 2009, 4, e4525.	1.1	105
119	Statistical data processing in clinical proteomics. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2008, 866, 77-88.	1.2	60
120	Assessment of PLSDA cross validation. <i>Metabolomics</i> , 2008, 4, 81-89.	1.4	1,178
121	Discriminant Q2 (DQ2) for improved discrimination in PLSDA models. <i>Metabolomics</i> , 2008, 4, 293-296.	1.4	69
122	PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data. <i>Journal of Chemometrics</i> , 2008, 22, 114-121.	0.7	52
123	Estimating kinetic parameters of complex catalytic reactions using a curve resolution based method. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2008, 91, 101-109.	1.8	7
124	The geometry of ASCA. <i>Journal of Chemometrics</i> , 2008, 22, 464-471.	0.7	19
125	Biomarkers for lysosomal storage disorders: identification and application as exemplified by chitotriosidase in Gaucher disease. <i>Acta Paediatrica, International Journal of Paediatrics</i> , 2008, 97, 7-14.	0.7	60
126	Optimized Time Alignment Algorithm for LC-MS Data: Correlation Optimized Warping Using Component Detection Algorithm-Selected Mass Chromatograms. <i>Analytical Chemistry</i> , 2008, 80, 7012-7021.	3.2	79

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127	Variable Selection Methods as a Tool To Find Sensor Locations for Distributed Parameter Systems. <i>Industrial & Engineering Chemistry Research</i> , 2008, 47, 1184-1191.	1.8	6
128	Multilevel Data Analysis of a Crossover Designed Human Nutritional Intervention Study. <i>Journal of Proteome Research</i> , 2008, 7, 4483-4491.	1.8	158
129	A Classification Model for the Leiden Proteomics Competition. <i>Statistical Applications in Genetics and Molecular Biology</i> , 2008, 7, Article8.	0.2	19
130	Simplivariate Models: Ideas and First Examples. <i>PLoS ONE</i> , 2008, 3, e3259.	1.1	16
131	Discovering gene expression patterns in time course microarray experiments by ANOVAâ€“SCA. <i>Bioinformatics</i> , 2007, 23, 1792-1800.	1.8	80
132	Manufacturing Vaccines: An Illustration of Using PAT Tools for Controlling the Cultivation of <i>Bordetella pertussis</i> . <i>Quality Engineering</i> , 2007, 19, 373-384.	0.7	8
133	Atherosclerosis and liver inflammation induced by increased dietary cholesterol intake: a combined transcriptomics and metabolomics analysis. <i>Genome Biology</i> , 2007, 8, R200.	13.9	210
134	Grey component analysis. <i>Journal of Chemometrics</i> , 2007, 21, 474-485.	0.7	19
135	Assessing the statistical validity of proteomics based biomarkers. <i>Analytica Chimica Acta</i> , 2007, 592, 210-217.	2.6	166
136	How to distinguish healthy from diseased? Classification strategy for mass spectrometryâ€“based clinical proteomics. <i>Proteomics</i> , 2007, 7, 3672-3680.	1.3	49
137	Statistical validation of megavariable effects in ASCA. <i>BMC Bioinformatics</i> , 2007, 8, 322.	1.2	137
138	Estimating confidence intervals for principal component loadings: A comparison between the bootstrap and asymptotic results. <i>British Journal of Mathematical and Statistical Psychology</i> , 2007, 60, 295-314.	1.0	67
139	Proposed minimum reporting standards for data analysis in metabolomics. <i>Metabolomics</i> , 2007, 3, 231-241.	1.4	361
140	A comparison of various methods for multivariate regression with highly collinear variables. <i>Statistical Methods and Applications</i> , 2007, 16, 193-228.	0.7	70
141	Large-Scale Human Metabolomics Studies: A Strategy for Data (Pre-) Processing and Validation. <i>Analytical Chemistry</i> , 2006, 78, 567-574.	3.2	744
142	A Theoretical Framework for Real Time Release with NIR and Chemometrics. <i>NIR News</i> , 2006, 17, 4-6.	1.6	2
143	Performance assessment and improvement of control charts for statistical batch process monitoring. <i>Statistica Neerlandica</i> , 2006, 60, 339-360.	0.9	14
144	Single channel event (SCE) for managing sensor failures in MSPC. <i>Computers and Chemical Engineering</i> , 2006, 30, 961-969.	2.0	3

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145	Assessing the performance of statistical validation tools for megavariable metabolomics data. <i>Metabolomics</i> , 2006, 2, 53-61.	1.4	138
146	Centering, scaling, and transformations: improving the biological information content of metabolomics data. <i>BMC Genomics</i> , 2006, 7, 142.	1.2	1,836
147	Linking PCA and time derivatives of dynamic systems. <i>Journal of Chemometrics</i> , 2006, 20, 43-53.	0.7	4
148	Maximum likelihood scaling (MALS). <i>Journal of Chemometrics</i> , 2006, 20, 120-127.	0.7	9
149	Fault detection properties of global, local and time evolving models for batch process monitoring. <i>Journal of Process Control</i> , 2005, 15, 799-805.	1.7	60
150	Multilevel component analysis of time-resolved metabolic fingerprinting data. <i>Analytica Chimica Acta</i> , 2005, 530, 173-183.	2.6	96
151	Symbiosis of chemometrics and metabolomics: past, present, and future. <i>Journal of Chemometrics</i> , 2005, 19, 376-386.	0.7	111
152	ASCA: analysis of multivariate data obtained from an experimental design. <i>Journal of Chemometrics</i> , 2005, 19, 469-481.	0.7	201
153	ANOVA-simultaneous component analysis (ASCA): a new tool for analyzing designed metabolomics data. <i>Bioinformatics</i> , 2005, 21, 3043-3048.	1.8	552
154	Tackling Calibration Problems of Spectroscopic Analysis in High-Throughput Experimentation. <i>Analytical Chemistry</i> , 2005, 77, 2227-2234.	3.2	8
155	Profiling of Liquid Crystal Displays with Raman Spectroscopy: Preprocessing of Spectra. <i>Applied Spectroscopy</i> , 2005, 59, 267-274.	1.2	8
156	Fusion of Mass Spectrometry-Based Metabolomics Data. <i>Analytical Chemistry</i> , 2005, 77, 6729-6736.	3.2	290
157	Analysis of longitudinal metabolomics data. <i>Bioinformatics</i> , 2004, 20, 2438-2446.	1.8	74
158	The effect of the size of the training set and number of principal components on the false alarm rate in statistical process monitoring. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2004, 73, 181-187.	1.8	35
159	Performance Optimization of Spectroscopic Process Analyzers. <i>Analytical Chemistry</i> , 2004, 76, 2656-2663.	3.2	18
160	Centering and scaling in component analysis. <i>Journal of Chemometrics</i> , 2003, 17, 16-33.	0.7	327
161	A framework for sequential multiblock component methods. <i>Journal of Chemometrics</i> , 2003, 17, 323-337.	0.7	190
162	Dynamic time warping of spectroscopic BATCH data. <i>Analytica Chimica Acta</i> , 2003, 498, 133-153.	2.6	74

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163	Quantitative analysis of target components by comprehensive two-dimensional gas chromatography. <i>Journal of Chromatography A</i> , 2003, 1019, 15-29.	1.8	110
164	Near-Infrared Spectroscopic Monitoring of a Series of Industrial Batch Processes Using a Bilinear Grey Model. <i>Applied Spectroscopy</i> , 2003, 57, 1007-1019.	1.2	18
165	An introduction to Multi-block Component Analysis by means of a flavor language case study. <i>Food Quality and Preference</i> , 2003, 14, 497-506.	2.3	13
166	Kinetic and mechanistic studies on the Heck reaction using real-time near infrared spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4455-4460.	1.3	12
167	A Systematic Quantification of the Sources of Variation of Process Analytical Measurements in the Steel Industry. <i>Quality Engineering</i> , 2003, 15, 391-402.	0.7	0
168	Peer Reviewed: How to Choose the Right Process Analyzer. <i>Analytical Chemistry</i> , 2002, 74, 368 A-373 A.	3.2	8
169	Selection of Optimal Process Analyzers for Plant-Wide Monitoring. <i>Analytical Chemistry</i> , 2002, 74, 3105-3111.	3.2	17
170	Direct sampling tandem mass spectrometry (MS/MS) and multiway calibration for isomer quantitation. <i>Analyst</i> , The, 2002, 127, 1054-1060.	1.7	26
171	Monitoring of batch processes using spectroscopy. <i>AIChE Journal</i> , 2002, 48, 2283-2297.	1.8	53
172	Constrained least squares methods for estimating reaction rate constants from spectroscopic data. <i>Journal of Chemometrics</i> , 2002, 16, 28-40.	0.7	23
173	Maximum likelihood fitting using ordinary least squares algorithms. <i>Journal of Chemometrics</i> , 2002, 16, 387-400.	0.7	85
174	Non-triviality and identification of a constrained Tucker3 analysis. <i>Journal of Chemometrics</i> , 2002, 16, 609-612.	0.7	29
175	Critical evaluation of approaches for on-line batch process monitoring. <i>Chemical Engineering Science</i> , 2002, 57, 3979-3991.	1.9	110
176	Determination of Rate Constants in Second-Order Kinetics Using UV-Visible Spectroscopy. <i>Applied Spectroscopy</i> , 2001, 55, 77-83.	1.2	33
177	Optimizing Meta-Parameters in Continuous Piecewise Direct Standardization. <i>Applied Spectroscopy</i> , 2001, 55, 458-466.	1.2	18
178	On the difference between low-rank and subspace approximation: improved model for multi-linear PLS regression. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2001, 58, 3-13.	1.8	56
179	A comparison of multiway regression and scaling methods. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2001, 59, 121-136.	1.8	79
180	Deflation in multiblock PLS. <i>Journal of Chemometrics</i> , 2001, 15, 485-493.	0.7	81

#	ARTICLE	IF	CITATIONS
181	Reply to 'Comment on a recently proposed resampling method'. Journal of Chemometrics, 2001, 15, 189-192.	0.7	4
182	Sufficient conditions for unique solutions within a certain class of curve resolution models. Journal of Chemometrics, 2001, 15, 405-411.	0.7	28
183	Process analyzer location and performance assessment for optimal process monitoring. AIChE Journal, 2001, 47, 2503-2514.	1.8	5
184	Comments on three-way analyses used for batch process data. Journal of Chemometrics, 2001, 15, 19-27.	0.7	44
185	Modelling of spectroscopic batch process data using grey models to incorporate external information. Journal of Chemometrics, 2001, 15, 101-121.	0.7	38
186	Multiway multiblock component and covariates regression models. Journal of Chemometrics, 2000, 14, 301-331.	0.7	92
187	Standardized Q-statistic for improved sensitivity in the monitoring of residuals in MSPC. Journal of Chemometrics, 2000, 14, 335-349.	0.7	34
188	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
189	Estimating reaction rate constants: comparison between traditional curve fitting and curve resolution. Analytica Chimica Acta, 2000, 419, 197-207.	2.6	42
190	Generalized contribution plots in multivariate statistical process monitoring. Chemometrics and Intelligent Laboratory Systems, 2000, 51, 95-114.	1.8	440
191	Linear techniques to correct for temperature-induced spectral variation in multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2000, 51, 189-200.	1.8	78
192	Calibration and detailed analysis of second-order flow injection analysis data with rank overlap. Analytica Chimica Acta, 2000, 422, 21-36.	2.6	28
193	Identification and quantification of sources of variation in the analysis of steel. Fresenius' Journal of Analytical Chemistry, 2000, 368, 397-406.	1.5	1
194	Fast On-Line Analysis of Process Alkane Gas Mixtures by NIR Spectroscopy. Applied Spectroscopy, 2000, 54, 406-412.	1.2	9
195	Spectroscopic Monitoring of Batch Reactions for On-Line Fault Detection and Diagnosis. Analytical Chemistry, 2000, 72, 5322-5330.	3.2	31
196	Correction of Temperature-Induced Spectral Variation by Continuous Piecewise Direct Standardization. Analytical Chemistry, 2000, 72, 1639-1644.	3.2	92
197	Calibration methods for complex second-order data. Analytica Chimica Acta, 1999, 398, 237-251.	2.6	69
198	Application of curve resolution based methods to kinetic data. Analytica Chimica Acta, 1999, 396, 231-240.	2.6	51

#	ARTICLE	IF	CITATIONS
199	Monitoring and diagnosing batch processes with multiway covariates regression models. <i>AICHE Journal</i> , 1999, 45, 1504-1520.	1.8	53
200	Multiway covariates regression models. <i>Journal of Chemometrics</i> , 1999, 13, 31-48.	0.7	35
201	Applications and new developments of the direct exponential curve resolution algorithm (DECRA). Examples of spectra and magnetic resonance images. <i>Journal of Chemometrics</i> , 1999, 13, 95-110.	0.7	39
202	Estimating rate constants and pure UV-vis spectra of a two-step reaction using trilinear models. <i>Journal of Chemometrics</i> , 1999, 13, 311-329.	0.7	67
203	Cross-validation of multiway component models. <i>Journal of Chemometrics</i> , 1999, 13, 491-510.	0.7	56
204	Monitoring a PVC Batch Process with Multivariate Statistical Process Control Charts. <i>Industrial & Engineering Chemistry Research</i> , 1999, 38, 4769-4776.	1.8	39
205	Rapid estimation of rate constants using on-line SW-NIR and trilinear models. <i>Analytica Chimica Acta</i> , 1998, 376, 339-355.	2.6	41
206	A multiway 3D QSAR analysis of a series of (S)-N-[(1-ethyl-2-pyrrolidiny]methyl]-6-methoxybenzamides. <i>Journal of Computer-Aided Molecular Design</i> , 1998, 12, 81-93.	1.3	23
207	Rapid estimation of rate constants of batch processes using on-line SW-NIR. <i>AICHE Journal</i> , 1998, 44, 2713-2723.	1.8	36
208	Constrained three-mode factor analysis as a tool for parameter estimation with second-order instrumental data. <i>Journal of Chemometrics</i> , 1998, 12, 125-147.	0.7	51
209	Influence of Temperature on Vibrational Spectra and Consequences for the Predictive Ability of Multivariate Models. <i>Analytical Chemistry</i> , 1998, 70, 1761-1767.	3.2	204
210	GRID/GOLPE 3D Quantitative Structure-Activity Relationship Study on a Set of Benzamides and Naphthamides, with Affinity for the Dopamine D3Receptor Subtype. <i>Journal of Medicinal Chemistry</i> , 1997, 40, 833-840.	2.9	34
211	Comments on multilinear PLS. <i>Journal of Chemometrics</i> , 1997, 11, 367-377.	0.7	85
212	Multiway calibration in 3D QSAR. <i>Journal of Chemometrics</i> , 1997, 11, 511-524.	0.7	59
213	Multivariate quality assessment of aged RP-HPLC columns. <i>Journal of Chemometrics</i> , 1996, 10, 351-370.	0.7	6
214	Chapter 12 Multivariate characterization of RP-HPLC stationary phases. <i>Journal of Chromatography Library</i> , 1995, 57, 403-449.	0.1	3
215	Selectivity, local rank, three-way data analysis and ambiguity in multivariate curve resolution. <i>Journal of Chemometrics</i> , 1995, 9, 31-58.	0.7	868
216	Some theoretical results on second-order calibration methods for data with and without rank overlap. <i>Journal of Chemometrics</i> , 1995, 9, 179-195.	0.7	48

#	ARTICLE	IF	CITATIONS
217	Online Detection and Identification Interferents in Multivariate Predictions of Organic Gases Using FT-IR Spectroscopy. <i>Analytical Chemistry</i> , 1995, 67, 2170-2179.	3.2	25
218	Theory of medium-rank second-order calibration with restricted-Tucker models. <i>Journal of Chemometrics</i> , 1994, 8, 21-36.	0.7	87
219	Three-way analyses problems and prospects. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1992, 15, 143-157.	1.8	161
220	Simple validity tools for judging the predictive performance of parafac and three-way PLS. <i>Journal of Chemometrics</i> , 1992, 6, 11-28.	0.7	17
221	Three-way methods for the calibration of chromatographic systems: Comparing PARAFAC and three-way PLS. <i>Journal of Chemometrics</i> , 1991, 5, 345-360.	0.7	75
222	Multivariate calibration of reversed-phase chromatographic systems. Some designs based on three-way data analysis. <i>Analytica Chimica Acta</i> , 1990, 235, 41-51.	2.6	20
223	Characterization of stationary/mobile phase combinations by using markers. <i>Analytica Chimica Acta</i> , 1988, 212, 95-104.	2.6	9