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List of Publications by Year in descending order

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234 papers	28,718 citations	13865 67 h-index	5539 163 g-index
243 all docs	243 docs citations	243 times ranked	17565 citing authors

#	Article	IF	Citations
1	PARAFAC. Tutorial and applications. Chemometrics and Intelligent Laboratory Systems, 1997, 38, 149-171.	3.5	2,318
2	Characterizing dissolved organic matter fluorescence with parallel factor analysis: a tutorial. Limnology and Oceanography: Methods, 2008, 6, 572-579.	2.0	1,969
3	Tracing dissolved organic matter in aquatic environments using a new approach to fluorescence spectroscopy. Marine Chemistry, 2003, 82, 239-254.	2.3	1,598
4	Fluorescence spectroscopy and multi-way techniques. PARAFAC. Analytical Methods, 2013, 5, 6557.	2.7	1,349
5	A new efficient method for determining the number of components in PARAFAC models. Journal of Chemometrics, 2003, 17, 274-286.	1.3	1,053
6	The N-way Toolbox for MATLAB. Chemometrics and Intelligent Laboratory Systems, 2000, 52, 1-4.	3.5	1,010
7	A fast non-negativity-constrained least squares algorithm. Journal of Chemometrics, 1997, 11, 393-401.	1.3	699
8	OpenFluorâ€“ an online spectral library of auto-fluorescence by organic compounds in the environment. Analytical Methods, 2014, 6, 658-661.	2.7	676
9	Multiway calibration. Multilinear PLS. Journal of Chemometrics, 1996, 10, 47-61.	1.3	666
10	Variable selection in regressionâ€”a tutorial. Journal of Chemometrics, 2010, 24, 728-737.	1.3	540
11	Practical aspects of PARAFAC modeling of fluorescence excitation-emission data. Journal of Chemometrics, 2003, 17, 200-215.	1.3	517
12	On the uniqueness of multilinear decomposition ofN-way arrays. Journal of Chemometrics, 2000, 14, 229-239.	1.3	489
13	Parallel factor analysis in sensor array processing. IEEE Transactions on Signal Processing, 2000, 48, 2377-2388.	5.3	481
14	Blind PARAFAC receivers for DS-CDMA systems. IEEE Transactions on Signal Processing, 2000, 48, 810-823.	5.3	449
15	Handling of Rayleigh and Raman scatter for PARAFAC modeling of fluorescence data using interpolation. Journal of Chemometrics, 2006, 20, 99-105.	1.3	434
16	Multiway calibration. Multilinear PLS. Journal of Chemometrics, 1996, 10, 47-61.	1.3	390
17	PARAFAC2â€”Part I. A direct fitting algorithm for the PARAFAC2 model. Journal of Chemometrics, 1999, 13, 275-294.	1.3	350
18	Centering and scaling in component analysis. Journal of Chemometrics, 2003, 17, 16-33.	1.3	327

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19	A comparison of algorithms for fitting the PARAFAC model. Computational Statistics and Data Analysis, 2006, 50, 1700-1734.	1.2	316
20	PARAFAC2â€"Part II. Modeling chromatographic data with retention time shifts. Journal of Chemometrics, 1999, 13, 295-309.	1.3	277
21	Cross-validation of component models: A critical look at current methods. Analytical and Bioanalytical Chemistry, 2008, 390, 1241-1251.	3.7	269
22	Multivariate Autofluorescence of Intact Food Systems. Chemical Reviews, 2006, 106, 1979-1994.	47.7	262
23	Automated alignment of chromatographic data. Journal of Chemometrics, 2006, 20, 484-497.	1.3	246
24	Fluorescence spectroscopy coupled with PARAFAC and PLS DA for characterization and classification of honey. Food Chemistry, 2015, 175, 284-291.	8.2	234
25	Dissolved Organic Matter Characterization Using Multiway Spectral Decomposition of Fluorescence Landscapes. Soil Science Society of America Journal, 2006, 70, 2028-2037.	2.2	233
26	Gas chromatography â€" mass spectrometry data processing made easy. Journal of Chromatography A, 2017, 1503, 57-64.	3.7	218
27	Multiway analysis of epilepsy tensors. Bioinformatics, 2007, 23, i10-i18.	4.1	210
28	Recent developments in CANDECOMP/PARAFAC algorithms: a critical review. Chemometrics and Intelligent Laboratory Systems, 2003, 65, 119-137.	3.5	208
29	From K-Means to Higher-Way Co-Clustering: Multilinear Decomposition With Sparse Latent Factors. IEEE Transactions on Signal Processing, 2013, 61, 493-506.	5.3	206
30	PARAFAC and missing values. Chemometrics and Intelligent Laboratory Systems, 2005, 75, 163-180.	3.5	202
31	Review on Multiway Analysis in Chemistryâ€"2000â€"2005. Critical Reviews in Analytical Chemistry, 2006, 36, 279-293.	3.5	197
32	Exploratory study of sugar production using fluorescence spectroscopy and multi-way analysis. Chemometrics and Intelligent Laboratory Systems, 1999, 46, 133-147.	3.5	196
33	Some common misunderstandings in chemometrics. Journal of Chemometrics, 2010, 24, 558-564.	1.3	196
34	Parallel Factor Analysis of Excitationâ€"Emission Matrix Fluorescence Spectra of Water Soluble Soil Organic Matter as Basis for the Determination of Conditional Metal Binding Parameters. Environmental Science & Technology, 2008, 42, 186-192.	10.0	191
35	Characterizing dissolved organic matter fluorescence with parallel factor analysis: a tutorial. Limnology and Oceanography: Methods, 2008, 6, 572-579.	2.0	189
36	Multivariate calibration. Analytica Chimica Acta, 2003, 500, 185-194.	5.4	181

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37	ChroMATHography: Solving Chromatographic Issues with Mathematical Models and Intuitive Graphics. Chemical Reviews, 2010, 110, 4582-4605.	47.7	173
38	Chemometrics in food scienceâ€"a demonstration of the feasibility of a highly exploratory, inductive evaluation strategy of fundamental scientific significance. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 31-60.	3.5	148
39	Least squares algorithms under unimodality and non-negativity constraints. Journal of Chemometrics, 1998, 12, 223-247.	1.3	145
40	Near-infrared chemical imaging (NIR-CI) on pharmaceutical solid dosage formsâ€"Comparing common calibration approaches. Journal of Pharmaceutical and Biomedical Analysis, 2008, 48, 554-561.	2.8	134
41	Solving GC-MS problems with PARAFAC2. TrAC - Trends in Analytical Chemistry, 2008, 27, 714-725.	11.4	134
42	Robust methods for multivariate data analysis. Journal of Chemometrics, 2005, 19, 549-563.	1.3	128
43	Improving the speed of multi-way algorithms:. Chemometrics and Intelligent Laboratory Systems, 1998, 42, 93-103.	3.5	114
44	Resolving the sign ambiguity in the singular value decomposition. Journal of Chemometrics, 2008, 22, 135-140.	1.3	114
45	Standard error of prediction for multiway PLS. Chemometrics and Intelligent Laboratory Systems, 2002, 61, 133-149.	3.5	104
46	Jack-knife technique for outlier detection and estimation of standard errors in PARAFAC models. Chemometrics and Intelligent Laboratory Systems, 2003, 65, 35-49.	3.5	98
47	Review of Chemometrics Applied to Spectroscopy: 1985-95, Part I. Applied Spectroscopy Reviews, 1996, 31, 73-124.	6.7	97
48	A fast non-negativity-constrained least squares algorithm. Journal of Chemometrics, 1997, 11, 393-401.	1.3	96
49	Modeling multiâ€way data with linearly dependent loadings. Journal of Chemometrics, 2009, 23, 324-340.	1.3	92
50	Data Fusion in Metabolomics Using Coupled Matrix and Tensor Factorizations. Proceedings of the IEEE, 2015, 103, 1602-1620.	21.3	92
51	Structure-revealing data fusion. BMC Bioinformatics, 2014, 15, 239.	2.6	91
52	Exploring the phenotypic expression of a regulatory proteome-altering gene by spectroscopy and chemometrics. Analytica Chimica Acta, 2001, 446, 169-184.	5.4	90
53	Pre-whitening of data by covariance-weighted pre-processing. Journal of Chemometrics, 2003, 17, 153-165.	1.3	88
54	Quantitative analysis of NMR spectra with chemometrics. Journal of Magnetic Resonance, 2008, 190, 26-32.	2.1	87

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55	A tutorial on the Lasso approach to sparse modeling. Chemometrics and Intelligent Laboratory Systems, 2012, 119, 21-31.	3.5	86
56	Maximum likelihood fitting using ordinary least squares algorithms. Journal of Chemometrics, 2002, 16, 387-400.	1.3	85
57	A modification of canonical variates analysis to handle highly collinear multivariate data. Journal of Chemometrics, 2006, 20, 425-435.	1.3	85
58	Orthogonal signal correction, wavelet analysis, and multivariate calibration of complicated process fluorescence data. Analytica Chimica Acta, 2000, 420, 181-195.	5.4	83
59	Improving the speed of multiway algorithms. Chemometrics and Intelligent Laboratory Systems, 1998, 42, 105-113.	3.5	82
60	Towards Rapid and Unique Curve Resolution of Low-Field NMR Relaxation Data: Trilinear SLICING versus Two-Dimensional Curve Fitting. Journal of Magnetic Resonance, 2002, 157, 141-155.	2.1	81
61	Understanding data fusion within the framework of coupled matrix and tensor factorizations. Chemometrics and Intelligent Laboratory Systems, 2013, 129, 53-63.	3.5	80
62	Recent chemometrics advances for foodomics. TrAC - Trends in Analytical Chemistry, 2017, 96, 42-51.	11.4	80
63	A comparison of multiway regression and scaling methods. Chemometrics and Intelligent Laboratory Systems, 2001, 59, 121-136.	3.5	79
64	First order Rayleigh scatter as a separate component in the decomposition of fluorescence landscapes. Analytica Chimica Acta, 2005, 537, 349-358.	5.4	73
65	Common and distinct components in data fusion. Journal of Chemometrics, 2017, 31, e2900.	1.3	71
66	Calibration methods for complex second-order data. Analytica Chimica Acta, 1999, 398, 237-251.	5.4	69
67	Application of N-PLS to gas chromatographic and sensory data of traditional balsamic vinegars of modena. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 54-65.	3.5	68
68	Multivariate data analysis as a tool in advanced quality monitoring in the food production chain. Trends in Food Science and Technology, 2002, 13, 235-244.	15.1	67
69	Handling within run retention time shifts in two-dimensional chromatography data using shift correction and modeling. Journal of Chromatography A, 2009, 1216, 4020-4029.	3.7	66
70	Using deep learning to evaluate peaks in chromatographic data. Talanta, 2019, 204, 255-260.	5.5	65
71	Analysis of lipoproteins using 2D diffusion-edited NMR spectroscopy and multi-way chemometrics. Analytica Chimica Acta, 2005, 531, 209-216.	5.4	64
72	Olive oil quantification of edible vegetable oil blends using triacylglycerols chromatographic fingerprints and chemometric tools. Talanta, 2011, 85, 177-182.	5.5	63

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73	Combining PARAFAC Analysis of HPLC-PDA Profiles and Structural Characterization Using HPLC-PDA-SPE-NMR-MS Experiments:â€‰Commercial Preparations of St. John's Wort. Analytical Chemistry, 2008, 80, 1978-1987.	6.5	62
74	Quantifying catecholamines using multi-way kinetic modelling. Analytica Chimica Acta, 2003, 475, 137-150.	5.4	61
75	Solving fundamental problems in chromatographic analysis. Analytical and Bioanalytical Chemistry, 2008, 390, 281-285.	3.7	58
76	Classification of GCâ€MS measurements of wines by combining data dimension reduction and variable selection techniques. Journal of Chemometrics, 2008, 22, 457-463.	1.3	58
77	EEMizer: Automated modeling of fluorescence EEM data. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 86-92.	3.5	57
78	Review of Chemometrics Applied to Spectroscopy: 1985-95, Part 2. Applied Spectroscopy Reviews, 1996, 31, 347-368.	6.7	56
79	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.	3.5	56
80	Multiblock variance partitioning: A new approach for comparing variation in multiple data blocks. Analytica Chimica Acta, 2008, 615, 18-29.	5.4	56
81	Forecasting individual breast cancer risk using plasma metabolomics and biocontours. Metabolomics, 2015, 11, 1376-1380.	3.0	54
82	Theory of net analyte signal vectors in inverse regression. Journal of Chemometrics, 2003, 17, 646-652.	1.3	53
83	Multi-way prediction in the presence of uncalibrated interferents. Journal of Chemometrics, 2007, 21, 76-86.	1.3	53
84	Review of Chemometrics Applied to Spectroscopy: 1985-95, Part 3 â€” Multi-way Analysis. Applied Spectroscopy Reviews, 1997, 32, 237-261.	6.7	52
85	PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data. Journal of Chemometrics, 2008, 22, 114-121.	1.3	52
86	Variable selection in multi-block regression. Chemometrics and Intelligent Laboratory Systems, 2016, 156, 89-101.	3.5	52
87	Emerging patterns in the global distribution of dissolved organic matter fluorescence. Analytical Methods, 2019, 11, 888-893.	2.7	52
88	A novel strategy for solving matrix effect in three-way data using parallel profiles with linear dependencies. Analytica Chimica Acta, 2007, 584, 397-402.	5.4	50
89	Enzymatic browning of vegetables. Calibration and analysis of variance by multiway methods. Chemometrics and Intelligent Laboratory Systems, 1996, 34, 85-102.	3.5	49
90	A classification tool for N-way array based on SIMCA methodology. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 73-85.	3.5	49

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91	Data fusion in metabolomic cancer diagnostics. Metabolomics, 2013, 9, 3-8.	3.0	49
92	Determination of the Botanical Origin of Honey by Front-Face Synchronous Fluorescence Spectroscopy. Applied Spectroscopy, 2014, 68, 557-563.	2.2	49
93	Chemometric Analysis of Organic Matter Fluorescence. , 2014, , 339-375.		49
94	Diagnosing Latent Copper Deficiency in Intact Barley Leaves (Hordeum vulgare, L.) Using Near Infrared Spectroscopy. Journal of Agricultural and Food Chemistry, 2013, 61, 10901-10910.	5.2	47
95	Joint Tensor Factorization and Outlying Slab Suppression With Applications. IEEE Transactions on Signal Processing, 2015, 63, 6315-6328.	5.3	47
96	Spectral reflectance at subâ€leaf scale including the spatial distribution discriminating NPK stress characteristics in barley using multiway partial least squares regression. International Journal of Remote Sensing, 2007, 28, 943-962.	2.9	46
97	Analysis of sensory data of Aceto Balsamico Tradizionale di Modena (ABTM) of different ageing by application of PARAFAC models. Food Quality and Preference, 2006, 17, 419-428.	4.6	45
98	PARAFAC models of fluorescence data with scattering: A comparative study. Chemometrics and Intelligent Laboratory Systems, 2015, 142, 124-130.	3.5	45
99	Active Photosensitizers in Butter Detected by Fluorescence Spectroscopy and Multivariate Curve Resolution. Journal of Agricultural and Food Chemistry, 2006, 54, 10197-10204.	5.2	43
100	Loopy MSC: A Simple Way to Improve Multiplicative Scatter Correction. Applied Spectroscopy, 2008, 62, 1153-1159.	2.2	41
101	Fluorescence spectroscopy as a potential metabonomic tool for early detection of colorectal cancer. Metabolomics, 2012, 8, 111-121.	3.0	40
102	The Use of Visible and Near-Infrared Reflectance Measurements to assess Sensory Changes in Carrot Texture and Sweetness during Heat Treatment. Biosystems Engineering, 2003, 85, 213-225.	4.3	39
103	A new approach for modelling sensor based data. Sensors and Actuators B: Chemical, 2005, 106, 719-729.	7.8	39
104	PowerSlicing. Journal of Magnetic Resonance, 2003, 163, 192-197.	2.1	38
105	Comparison of PARAFAC2 and MCR-ALS for resolution of an analytical liquid dilution system. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 13-25.	3.5	38
106	Multiâ€way models for sensory profiling data. Journal of Chemometrics, 2008, 22, 36-45.	1.3	38
107	Core consistency diagnostic in PARAFAC2. Journal of Chemometrics, 2013, 27, 99-105.	1.3	38
108	Univariate and multivariate modelling of flavour release in chewing gum using time-intensity: a comparison of data analytical methods. Food Quality and Preference, 2005, 16, 327-343.	4.6	37

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109	Real-time monitoring and chemical profiling of a cultivation process. Chemometrics and Intelligent Laboratory Systems, 2006, 84, 106-113.	3.5	37
110	A comparison of a common approach to partial least squares-discriminant analysis and classical least squares in hyperspectral imaging. International Journal of Pharmaceutics, 2009, 373, 179-182.	5.2	37
111	Exploring Fluorescence Spectra of Apple Juice and Their Connection to Quality Parameters by Chemometrics. Journal of Agricultural and Food Chemistry, 1996, 44, 3202-3205.	5.2	36
112	PLS works. Journal of Chemometrics, 2009, 23, 69-71.	1.3	36
113	Extension of SO-PLS to multi-way arrays: SO-N-PLS. Chemometrics and Intelligent Laboratory Systems, 2017, 164, 113-126.	3.5	36
114	Benchmarking support vector regression against partial least squares regression and artificial neural network: Effect of sample size on model performance. Journal of Near Infrared Spectroscopy, 2017, 25, 381-390.	1.5	36
115	Fluorescence spectroscopy and chemometrics for classification of breast cancer samplesâ€"a feasibility study using extended canonical variates analysis. Journal of Chemometrics, 2007, 21, 451-458.	1.3	35
116	Data Pre-processing. , 2009, , 29-50.		34
117	Multiscale entropy analysis of resting-state magnetoencephalogram with tensor factorisations in Alzheimer's disease. Brain Research Bulletin, 2015, 119, 136-144.	3.0	34
118	Using PAT to accelerate the transition to continuous API manufacturing. Analytical and Bioanalytical Chemistry, 2017, 409, 821-832.	3.7	34
119	Temperature-induced variation for NIR tensor-based calibration. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 75-82.	3.5	33
120	Discriminating olive and non-olive oils using HPLC-CAD and chemometrics. Analytical and Bioanalytical Chemistry, 2011, 399, 2083-2092.	3.7	33
121	Coclusteringâ€"a useful tool for chemometrics. Journal of Chemometrics, 2012, 26, 256-263.	1.3	33
122	Multiway chemometric analysis of the metabolic response to toxins monitored by NMR. Chemometrics and Intelligent Laboratory Systems, 2005, 76, 79-89.	3.5	32
123	Development of models for predicting toxicity from sediment chemistry by partial least squares-discriminant analysis and counter-propagation artificial neural networks. Environmental Pollution, 2010, 158, 607-614.	7.5	32
124	Mathematical chromatography solves the cocktail party effect in mixtures using 2D spectra and PARAFAC. TrAC - Trends in Analytical Chemistry, 2010, 29, 281-284.	11.4	32
125	USE OF PHYSICO-CHEMICAL METHODS FOR ASSESSMENT OF SENSORY CHANGES IN CARROT TEXTURE AND SWEETNESS DURING COOKING. Journal of Texture Studies, 2002, 33, 367-388.	2.5	31
126	Lameness detection challenges in automated milking systems addressed with partial least squares discriminant analysis. Journal of Dairy Science, 2014, 97, 7476-7486.	3.4	31

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127	Standard error of prediction for multilinear PLS. Chemometrics and Intelligent Laboratory Systems, 2005, 75, 69-76.	3.5	29
128	Finding relevant spectral regions between spectroscopic techniques by use of cross model validation and partial least squares regression. Analytica Chimica Acta, 2007, 595, 323-327.	5.4	29
129	Application of Support Vector Regression for Simultaneous Modelling of near Infrared Spectra from Multiple Process Steps. Journal of Near Infrared Spectroscopy, 2015, 23, 75-84.	1.5	28
130	Maternal obesity and offspring dietary patterns at 9 months of age. European Journal of Clinical Nutrition, 2015, 69, 668-675.	2.9	28
131	Exploring complex interactions in designed data using GEMANOVA. Color changes in fresh beef during storage. Journal of Chemometrics, 2002, 16, 294-304.	1.3	27
132	Automated resolution of overlapping peaks in chromatographic data. Journal of Chemometrics, 2014, 28, 71-82.	1.3	25
133	Least squares algorithms under unimodality and non-negativity constraints. Journal of Chemometrics, 1998, 12, 223-247.	1.3	25
134	Effects of windbreak strips of willow coppiceâ€"modelling and field experiment on barley in Denmark. Agriculture, Ecosystems and Environment, 2002, 93, 25-32.	5.3	23
135	Prediction of sensory quality in raw carrots (Daucus carota L.) using multi-block LS-ParPLS. Food Quality and Preference, 2008, 19, 609-617.	4.6	22
136	Chemometric quality control of chromatographic purity. Journal of Chromatography A, 2010, 1217, 6503-6510.	3.7	22
137	A chemometric approach to the environmental problem of predicting toxicity in contaminated sediments. Journal of Chemometrics, 2010, 24, 379-386.	1.3	21
138	Tucker core consistency for validation of restricted Tucker3 models. Analytica Chimica Acta, 2012, 723, 18-26.	5.4	21
139	Determination of the protein content in brine from salted herring using near-infrared spectroscopy. LWT - Food Science and Technology, 2004, 37, 803-809.	5.2	20
140	Practical comparison of multivariate chemometric techniques for pattern recognition used in environmental monitoring. Analytical Methods, 2012, 4, 676.	2.7	20
141	Classification Methods of Multiway Arrays as a Basic Tool for Food PDO Authentication. Comprehensive Analytical Chemistry, 2013, , 339-382.	1.3	20
142	An automated method for baseline correction, peak finding and peak grouping in chromatographic data. Analyst, The, 2013, 138, 3502.	3.5	20
143	Can We Trust Score Plots?. Metabolites, 2020, 10, 278.	2.9	20
144	Prediction of Polyphenol Oxidase Activity in Model Solutions Containing Various Combinations of Chlorogenic Acid, (â˜)-Epicatechin, O2, CO2, Temperature, and pH by Multiway Data Analysis. Journal of Agricultural and Food Chemistry, 1997, 45, 2399-2406.	5.2	19

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145	A metabolomic investigation of splanchnic metabolism using 1H NMR spectroscopy of bovine blood plasma. Analytica Chimica Acta, 2005, 536, 1-6.	5.4	19
146	Vibrational overtone combination spectroscopy (VOCSY)â€"a new way of using IR and NIR data. Analytical and Bioanalytical Chemistry, 2007, 388, 179-188.	3.7	19
147	Prediction of skin quality properties by different Multivariate Image Analysis methodologies. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 6-13.	3.5	19
148	Image analysis for maintenance of coating quality in nickel electroplating baths â€“ Real time control. Analytica Chimica Acta, 2011, 706, 1-7.	5.4	19
149	From untargeted chemical profiling to peak tables â€“ A fully automated AI driven approach to untargeted GC-MS. TrAC - Trends in Analytical Chemistry, 2021, 145, 116451.	11.4	19
150	Direct Measurement of Lipid Peroxidation in Oil-in-Water Emulsions Using Multiwavelength Derivative UV-Spectroscopy. Journal of Agricultural and Food Chemistry, 1997, 45, 1741-1745.	5.2	18
151	Calibration, standardization, and quantitative analysis of multidimensional fluorescence (MDF) measurements on complex mixtures (IUPAC Technical Report). Pure and Applied Chemistry, 2017, 89, 1849-1870.	1.9	18
152	Coupled Matrix Factorization with Sparse Factors to Identify Potential Biomarkers in Metabolomics. , 2012, , .		17
153	Structure-revealing data fusion model with applications in metabolomics. , 2013, 2013, 6023-6.		17
154	A Metabolomic Approach to Beer Characterization. Molecules, 2021, 26, 1472.	3.8	17
155	Classification of Membrane Permeability of Drug Candidates: A Methodological Investigation. QSAR and Combinatorial Science, 2005, 24, 449-457.	1.4	16
156	Multivariate evaluation of pharmacological responses in early clinical trials â€“ a study of rILâ€21 in the treatment of patients with metastatic melanoma. British Journal of Clinical Pharmacology, 2010, 69, 379-390.	2.4	16
157	Geometric search: A new approach for fitting PARAFAC2 models on GC-MS data. Talanta, 2018, 185, 378-386.	5.5	16
158	Laser-induced breakdown spectroscopy (LIBS) spectra interpretation and characterization using parallel factor analysis (PARAFAC): a new procedure for data and spectral interference processing fostering the waste electrical and electronic equipment (WEEE) recycling process. Journal of Analytical Atomic Spectrometry, 2020, 35, 1115-1124.	3.0	16
159	Mathematical programming algorithms for regression-based nonlinear filtering in R/sup N/. IEEE Transactions on Signal Processing, 1999, 47, 771-782.	5.3	15
160	Generalized correlation loadings. Chemometrics and Intelligent Laboratory Systems, 2006, 84, 119-125.	3.5	15
161	Application of Multi-Way Analysis to 2D NMR Data. Annual Reports on NMR Spectroscopy, 2006, 59, 207-233.	1.5	15
162	Seizure Recognition on Epilepsy Feature Tensor. Annual International Conference of the IEEE Engineering in Medicine and Biology Society, 2007, 2007, 4273-6.	0.5	15

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163	DoubleSlicing: A non-iterative single profile multi-exponential curve resolution procedure. Journal of Magnetic Resonance, 2007, 189, 286-292.	2.1	15
164	Flatbed scanners as a source of imaging. Brightness assessment and additives determination in a nickel electroplating bath. Analytica Chimica Acta, 2011, 694, 38-45.	5.4	15
165	Experienced and inexperienced observers achieved relatively high within-observer agreement on video mobility scoring of dairy cows. Journal of Dairy Science, 2015, 98, 4560-4571.	3.4	15
166	Untargeted Metabolomic Profile for the Detection of Prostate Carcinomaâ€"Preliminary Results from PARAFAC2 and PLSâ€"DA Models. Molecules, 2019, 24, 3063.	3.8	15
167	Application of Rotated PCA Models to Facilitate Interpretation of Metabolite Profiles: Commercial Preparations of St. Johnâ€™s Wort. Planta Medica, 2009, 75, 271-279.	1.3	14
168	Increasing Process Understanding by Analyzing Complex Interactions in Experimental Data. Journal of Pharmaceutical Sciences, 2009, 98, 1852-1861.	3.3	14
169	Feasibility of Serodiagnosis of Ovarian Cancer by Mass Spectrometry. Analytical Chemistry, 2009, 81, 1907-1913.	6.5	14
170	Comprehensive control charting applied to chromatography. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 215-225.	3.5	14
171	On the uniqueness of multilinear decomposition of N-way arrays. Journal of Chemometrics, 2000, 14, 229-239.	1.3	14
172	Exploratory study of winter wheat reflectance during vegetative growth using threeâ€mode component analysis. International Journal of Remote Sensing, 2006, 27, 919-937.	2.9	13
173	Nonnegative PARAFAC2: A Flexible Coupling Approach. Lecture Notes in Computer Science, 2018, , 89-98.	1.3	13
174	New exploratory clustering tool. Journal of Chemometrics, 2008, 22, 91-100.	1.3	12
175	Coupled Matrix Factorization with Sparse Factors to Identify Potential Biomarkers in Metabolomics. International Journal of Knowledge Discovery in Bioinformatics, 2012, 3, 22-43.	0.8	12
176	The effects of water and dairy drinks on dietary patterns in overweight adolescents. International Journal of Food Sciences and Nutrition, 2016, 67, 314-324.	2.8	12
177	Forecasting Chronic Diseases Using Data Fusion. Journal of Proteome Research, 2017, 16, 2435-2444.	3.7	12
178	SCREAM: A novel method for multi-way regression problems with shifts and shape changes in one mode. Chemometrics and Intelligent Laboratory Systems, 2013, 129, 64-75.	3.5	11
179	Accelerating PARAFAC2 algorithms for non-negative complex tensor decomposition. Chemometrics and Intelligent Laboratory Systems, 2021, 214, 104312.	3.5	11
180	A phenomenological study of ripening of salted herring. Assessing homogeneity of data from different countries and laboratories. Journal of Chemometrics, 2002, 16, 81-88.	1.3	10

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181	Quantification and handling of sampling errors in instrumental measurements: a case study. Chemometrics and Intelligent Laboratory Systems, 2004, 72, 43-50.	3.5	10
182	Data handling for interactive metabolomics: tools for studying the dynamics of metabolome-macromolecule interactions. Metabolomics, 2012, 8, 52-63.	3.0	10
183	Indicators of dietary patterns in Danish infants at 9 months of age. Food and Nutrition Research, 2015, 59, 27665.	2.6	10
184	Modeling Food Fluorescence with PARAFAC. Reviews in Fluorescence, 2018, , 161-197.	0.5	10
185	Fused adjacency matrices to enhance information extraction: The beer benchmark. Analytica Chimica Acta, 2019, 1061, 70-83.	5.4	10
186	Trusting our machines: validating machine learning models for single-molecule transport experiments. Chemical Society Reviews, 2022, 51, 6875-6892.	38.1	10
187	Dioxin screening in fish product by pattern recognition of biomarkers. Chemosphere, 2007, 67, S28-S35.	8.2	9
188	Direct functional assessment of the composite phenotype through multivariate projection strategies. Genomics, 2008, 92, 373-383.	2.9	9
189	Regional differences in world human body dimensions: the multi-way analysis approach. Theoretical Issues in Ergonomics Science, 2008, 9, 325-345.	1.8	9
190	Quantitative determination of additives in a commercial electroplatingnickel bath by spectrophotometry and multivariate analysis. Analytical Methods, 2010, 2, 86-92.	2.7	9
191	Multivariate interpretation of the urinary steroid profile and trainingâ€induced modifications. The case study of a Marathon runner. Drug Testing and Analysis, 2019, 11, 1556-1565.	2.6	9
192	Solving the sign indeterminacy for multiway models. Journal of Chemometrics, 2013, 27, 70-75.	1.3	8
193	Direct, simultaneous quantification of fructooligosaccharides by FT-MIR ATR spectroscopy and chemometrics for rapid identification of superior, engineered Î²-fructofuranosidases. Analytical and Bioanalytical Chemistry, 2015, 407, 1661-1671.	3.7	8
194	Attempt to separate the fluorescence spectra of adrenaline and noradrenaline using chemometrics. Luminescence, 2001, 16, 91-101.	2.9	7
195	CuBatch, a MATLABÂ® interface for n-mode data analysis. Chemometrics and Intelligent Laboratory Systems, 2005, 77, 122-130.	3.5	7
196	Chemometric approach to chromatic spatial variance. Case study: patchiness of the Skyros wall lizard. Journal of Chemometrics, 2012, 26, 246-255.	1.3	7
197	All sparse PCA models are wrong, but some are useful. Part II: Limitations and problems of deflation. Chemometrics and Intelligent Laboratory Systems, 2021, 208, 104212.	3.5	7
198	PARAFAC2 and local minima. Chemometrics and Intelligent Laboratory Systems, 2021, 219, 104446.	3.5	7

#	Article	IF	Citations
199	Application of Fuzzy Logic and Near Infrared Spectroscopy for Malt Quality Evaluation. Journal of the Institute of Brewing, 2002, 108, 444-451.	2.3	6
200	Rapid dioxin assessment in fish products by fatty acid pattern recognition. Analyst, The, 2004, 129, 553.	3.5	6
201	Multi-way analysis for investigation of industrial pectin using an analytical liquid dilution system. Chemometrics and Intelligent Laboratory Systems, 2006, 84, 9-20.	3.5	6
202	PowerSlicing to determine fluorescence lifetimes of water-soluble organic matter derived from soils, plant biomass, and animal manures. Analytical and Bioanalytical Chemistry, 2008, 390, 2189-2194.	3.7	6
203	Multilinear Models: Iterative Methods. , 2009, , 411-451.		6
204	Chemometric Analysis of NMR Spectra. , 2017, , 1-20.		6
205	Algorithm for finding an interpretable simple neural network solution using PLS. Journal of Chemometrics, 1995, 9, 423-430.	1.3	5
206	Modeling of Temperature-Induced Near-Infrared and Low-Field Time-Domain Nuclear Magnetic Resonance Spectral Variation: Chemometric Prediction of Limonene and Water Content in Spray-Dried Delivery Systems. Applied Spectroscopy, 2009, 63, 141-152.	2.2	5
207	Non-negative mixtures. , 2010, , 515-547.		5
208	A New Principle for Unique Spectral Decomposition of 2D NMR Data. Special Publication - Royal Society of Chemistry, 0, , 195-203.	0.0	5
209	PARASIAS: A new method for analyzing higher-order tensors with shifting profiles. Analytica Chimica Acta, 2023, 1238, 339848.	5.4	5
210	On communication diversity for blind identifiability and the uniqueness of low-rank decomposition of N-way arrays. , 0, , .		4
211	Quantifying and handling errors in instrumental measurements using the measurement error theory. Journal of Chemometrics, 2003, 17, 621-629.	1.3	4
212	Wheat flour formulation by mixture design and multivariate study of its technological properties. Journal of Chemometrics, 2010, 24, 523-533.	1.3	4
213	Using GEMANOVA to explore the pattern generating properties of the Deltaâ€Notch model. Journal of Chemometrics, 2010, 24, 626-634.	1.3	4
214	No genetic footprints of the fat mass and obesity associated (FTO) gene in human plasma 1H CPMG NMR metabolic profiles. Metabolomics, 2014, 10, 132-140.	3.0	4
215	A fast non-negativity-constrained least squares algorithm. , 1997, 11, 393.		4
216	Hierarchical classification models and Handheld NIR spectrometer to human blood stains identification on different floor tiles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120533.	3.9	4

#	Article	IF	Citations
217	Chemometric Analysis of NMR Spectra. , 2018, , 1649-1668.		3
218	PARAFAC2Â-ÂPart I. A direct fitting algorithm for the PARAFAC2 model. Journal of Chemometrics, 1999, 13, 275-294.	1.3	3
219	Development of Dietary Patterns Spanning Infancy and Toddlerhood: Relation to Body Size, Composition and Metabolic Risk Markers at Three Years. AIMS Public Health, 2015, 2, 332-357.	2.6	3
220	Automatic and non-targeted analysis of the volatile profile of natural and alkalized cocoa powders using SBSE-GC-MS and chemometrics. Food Chemistry, 2022, 389, 133074.	8.2	3
221	Least squares algorithms under unimodality and non-negativity constraints. , 1998, 12, 223.		2
222	Multivariate analysis of time domain NMR signals in relation to food quality. Special Publication - Royal Society of Chemistry, 0, , 239-254.	0.0	2
223	AlgorithmÂXXX: Concurrent Alternating Least Squares for multiple simultaneous Canonical Polyadic Decompositions. ACM Transactions on Mathematical Software, 0, , .	2.9	2
224	Special issue in honour of D. Luc Massart (1941â€“2005). Journal of Chemometrics, 2007, 21, 251-251.	1.3	1
225	In memory of Richard Harshman. Journal of Chemometrics, 2009, 23, 315-315.	1.3	1
226	An expert system for automated flavour matching â€“ Prioritizer. Flavour and Fragrance Journal, 2017, 32, 286-293.	2.6	1
227	Multilinear Models, Iterative Methods. , 2020, , 267-304.		1
228	Cross-product penalized component analysis (X-CAN). Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104038.	3.5	1
229	Spider web biomonitoring: A cost-effective source apportionment approach for urban particulate matter. Environmental Pollution, 2021, 286, 117328.	7.5	1
230	Who is winning? A comparison of humans versus computers for calibration model building. Journal of Chemometrics, 2021, 35, e3378.	1.3	1
231	Challenges for data analysis in flavour science. Developments in Food Science, 2006, 43, 619-621.	0.0	0
232	Regional differences in world human body dimensions: the multi-way analysis approach. Theoretical Issues in Ergonomics Science, 2008, 9, 477-477.	1.8	0
233	Calibration model fusion. Journal of Chemometrics, 2023, 37, e3350.	1.3	0
234	Accelerating Jackknife Resampling for the Canonical Polyadic Decomposition. Frontiers in Applied Mathematics and Statistics, 2022, 8, .	1.3	0