

Douglas Neil Rutledge

List of Publications by Year in descending order

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186
papers

5,615
citations

94381

37
h-index

110317

64
g-index

193
all docs

193
docs citations

193
times ranked

6559
citing authors

#	ARTICLE	IF	CITATIONS
1	A tutorial on the analysis of multifactorial designs from one or more data sources using AComDim. <i>Journal of Chemometrics</i> , 2023, 37, .	0.7	2
2	Discriminability and uncertainty in principal component analysis (PCA) of temporal check-all-that-apply (TCATA) data. <i>Food Quality and Preference</i> , 2022, 96, 104370.	2.3	10
3	Metataxonomics, metagenomics and metabolomics analysis of the influence of temperature modification in full-scale anaerobic digesters. <i>Bioresource Technology</i> , 2022, 346, 126612.	4.8	10
4	Pre-processing ensembles with response oriented sequential alternation calibration (PROSAC): A step towards ending the pre-processing search and optimization quest for near-infrared spectral modelling. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2022, 222, 104497.	1.8	11
5	Is the Calibration Transfer of Multivariate Calibration Models between High- and Low-Field NMR Instruments Possible? A Case Study of Lignin Molecular Weight. <i>Analytical Chemistry</i> , 2022, 94, 3997-4004.	3.2	8
6	Response oriented covariates selection (ROCS) for fast block order- and scale-independent variable selection in multi-block scenarios. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2022, , 104551.	1.8	3
7	A longitudinal study of the effect of temperature modification in full-scale anaerobic digesters â€“ dataset combining 16S rDNA gene sequencing, metagenomics, and metabolomics data. <i>Data in Brief</i> , 2022, 41, 107960.	0.5	0
8	Exogenous application of bioregulators in <i>Coffea arabica</i> beans during ripening: Investigation of UVâ€“Visible and NIR mixture design-fingerprints using AComDim-ICA. <i>Microchemical Journal</i> , 2022, 181, 107702.	2.3	2
9	FRUITNIR-GUI: A graphical user interface for correcting external influences in multi-batch near infrared experiments related to fruit quality prediction. <i>Postharvest Biology and Technology</i> , 2021, 175, 111414.	2.9	8
10	Parallel pre-processing through orthogonalization (PORTO) and its application to near-infrared spectroscopy. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 212, 104190.	1.8	21
11	Quantification of palm oil bioactive compounds by ultraâ€“highâ€“performance supercritical fluid chromatography and chemometrics. <i>Canadian Journal of Chemical Engineering</i> , 2021, , .	0.9	1
12	Urinary Medium-Chained Acyl-Carnitines Sign High Caloric Intake whereas Short-Chained Acyl-Carnitines Sign High -Protein Diet within a High-Fat, Hypercaloric Diet in a Randomized Crossover Design Dietary Trial. <i>Nutrients</i> , 2021, 13, 1191.	1.7	5
13	Raman Imaging and Chemometrics Evaluation of Natural and Synthetic Beeswaxes as Matrices for Nanostructured Lipid Carriers Development. <i>Brazilian Journal of Analytical Chemistry</i> , 2021, 8, .	0.3	3
14	Recent trends in multi-block data analysis in chemometrics for multi-source data integration. <i>TrAC - Trends in Analytical Chemistry</i> , 2021, 137, 116206.	5.8	86
15	Stability study of furans, glucose and xylose under overliming conditions: Effect of sugar degradation products. <i>Bioresource Technology Reports</i> , 2021, 15, 100722.	1.5	1
16	A short note on achieving similar performance to deep learning with practical chemometrics. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 214, 104336.	1.8	7
17	Complementary chemometrics and deep learning for semantic segmentation of tall and wide visible and near-infrared spectral images of plants. <i>Computers and Electronics in Agriculture</i> , 2021, 186, 106226.	3.7	15
18	Chemometric pre-processing can negatively affect the performance of near-infrared spectroscopy models for fruit quality prediction. <i>Talanta</i> , 2021, 229, 122303.	2.9	53

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19	Monte Carlo methods for estimating Mallows's Cp and AIC criteria for PLSR models. Illustration on agronomic spectroscopic NIR data. <i>Journal of Chemometrics</i> , 2021, 35, e3369.	0.7	4
20	Multiblock methods in Analytical Chemistry. <i>Brazilian Journal of Analytical Chemistry</i> , 2021, 8, 16-21.	0.3	0
21	A generic workflow combining deep learning and chemometrics for processing close-range spectral images to detect drought stress in <i>Arabidopsis thaliana</i> to support digital phenotyping. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 216, 104373.	1.8	9
22	Are standard sample measurements still needed to transfer multivariate calibration models between near-infrared spectrometers? The answer is not always. <i>TrAC - Trends in Analytical Chemistry</i> , 2021, 143, 116331.	5.8	39
23	Rearrangement of incomplete multi-omics datasets combined with ComDim for evaluating replicate cross-platform variability and batch influence. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 218, 104422.	1.8	3
24	Digital images and independent components analysis in the determination of bioactive compounds from grape juice. <i>LWT - Food Science and Technology</i> , 2021, 152, 112308.	2.5	4
25	Different Methods for Determining the Dimensionality of Multivariate Models. <i>Frontiers in Analytical Science</i> , 2021, 1, .	1.1	7
26	Independent components analysis (ICA) at the "cocktail-party" in analytical chemistry. <i>Talanta</i> , 2020, 208, 120451.	2.9	25
27	MBA-GUI: A chemometric graphical user interface for multi-block data visualisation, regression, classification, variable selection and automated pre-processing. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2020, 205, 104139.	1.8	36
28	Utilising variable sorting for normalisation to correct illumination effects in close-range spectral images of potato plants. <i>Biosystems Engineering</i> , 2020, 197, 318-323.	1.9	17
29	Multiblock modelling on the study of the kinetic degradation of rosuvastatin calcium in the presence of retention time shifts and rank deficiency. <i>Analytica Chimica Acta</i> , 2020, 1133, 77-87.	2.6	4
30	New data preprocessing trends based on ensemble of multiple preprocessing techniques. <i>TrAC - Trends in Analytical Chemistry</i> , 2020, 132, 116045.	5.8	173
31	Extraction of information about structural changes in a semisolid pharmaceutical formulation from near-infrared and Raman images by multivariate curve resolution "alternating least squares and ComDim. <i>Journal of Chemometrics</i> , 2020, 34, e3288.	0.7	5
32	Two standard-free approaches to correct for external influences on near-infrared spectra to make models widely applicable. <i>Postharvest Biology and Technology</i> , 2020, 170, 111326.	2.9	36
33	Molecular markers of dietary essential amino acid-deficiency. <i>Proceedings of the Nutrition Society</i> , 2020, 79, .	0.4	0
34	Assessment of the microbial interplay during anaerobic co-digestion of wastewater sludge using common components analysis. <i>PLoS ONE</i> , 2020, 15, e0232324.	1.1	18
35	SPORT pre-processing can improve near-infrared quality prediction models for fresh fruits and agro-materials. <i>Postharvest Biology and Technology</i> , 2020, 168, 111271.	2.9	48
36	Effect of ammonia exposure and acclimation on the performance and the microbiome of anaerobic digestion. <i>Bioresource Technology Reports</i> , 2020, 11, 100488.	1.5	10

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37	Pre-processing Methods. , 2020, , 1-75.		4
38	Changes in Red Wine Composition during Bottle Aging: Impacts of Grape Variety, Vineyard Location, Maturity, and Oxygen Availability during Aging. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 13331-13343.	2.4	13
39	Evaluation of the impact of buffered peptone water composition on the discrimination between <i>Salmonella enterica</i> and <i>Escherichia coli</i> by Raman spectroscopy. <i>Analytical and Bioanalytical Chemistry</i> , 2020, 412, 3595-3604.	1.9	6
40	Assessment of substrate biodegradability improvement in anaerobic Co-digestion using a chemometrics-based metabolomic approach. <i>Chemosphere</i> , 2020, 254, 126812.	4.2	11
41	Exploratory study on the possibility to link gasoline samples sharing a common source after alteration by evaporation or combustion. <i>Forensic Science International</i> , 2019, 301, 190-201.	1.3	8
42	ComDim Methods for the Analysis of Multiblock Data in a Data Fusion Perspective. <i>Data Handling in Science and Technology</i> , 2019, , 179-204.	3.1	17
43	Chemical Variability of the Essential Oil of <i>Origanum ehrenbergii</i> Boiss. from Lebanon, Assessed by Independent Component Analysis (ICA) and Common Component and Specific Weight Analysis (CCSWA). <i>International Journal of Molecular Sciences</i> , 2019, 20, 1026.	1.8	8
44	Molecular Markers of Dietary Essential Amino Acid-deficiency (P08-059-19). <i>Current Developments in Nutrition</i> , 2019, 3, nzz044.P08-059-19.	0.1	0
45	Automatic de-noising of close-range hyperspectral images with a wavelength-specific shearlet-based image noise reduction method. <i>Sensors and Actuators B: Chemical</i> , 2019, 281, 1034-1044.	4.0	27
46	Evaluation and validation of an analytical approach for high-throughput metabolomic fingerprinting using direct introduction high-resolution mass spectrometry: Applicability to classification of urine of scrapie-infected ewes. <i>European Journal of Mass Spectrometry</i> , 2019, 25, 251-258.	0.5	8
47	MATLAB in electrochemistry: A review. <i>Talanta</i> , 2019, 194, 205-225.	2.9	50
48	Evaluation of an untargeted chemometric approach for the source inference of ignitable liquids in forensic science. <i>Forensic Science International</i> , 2019, 295, 8-18.	1.3	17
49	Urinary Metabolomics Profiles Associated to Bovine Meat Ingestion in Humans. <i>Molecular Nutrition and Food Research</i> , 2019, 63, e1700834.	1.5	22
50	A variable selection method for multiclass classification problems using two-class ROC analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 177, 35-46.	1.8	18
51	An untargeted evaluation of food contact materials by flow injection analysis-mass spectrometry (FIA-MS) combined with independent components analysis (ICA). <i>Analytica Chimica Acta</i> , 2018, 1022, 81-88.	2.6	13
52	ComDim: From multiblock data analysis to path modeling. <i>Food Quality and Preference</i> , 2018, 67, 27-34.	2.3	27
53	Comparison of common components analysis with principal components analysis and independent components analysis: Application to SPME-GC-MS volatolomic signatures. <i>Talanta</i> , 2018, 178, 854-863.	2.9	35
54	Fluorescence spectroscopy coupled with independent components analysis to monitor molecular changes during heating and cooling of Cantal type cheeses with different NaCl and KCl contents. <i>Journal of the Science of Food and Agriculture</i> , 2018, 98, 963-975.	1.7	14

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55	Potential of dynamically harmonized Fourier transform ion cyclotron resonance cell for high-throughput metabolomics fingerprinting: control of data quality. <i>Analytical and Bioanalytical Chemistry</i> , 2018, 410, 483-490.	1.9	6
56	Determination of the optimal number of components in independent components analysis. <i>Talanta</i> , 2018, 179, 538-545.	2.9	25
57	Investigation of <i>Origanum libanoticum</i> Essential Oils Chemical Polymorphism by Independent Components Analysis (ICA). <i>Natural Product Communications</i> , 2018, 13, 1934578X1801301.	0.2	3
58	Comparison of different chemometric methods to extract chemical and physical information from Raman images of homogeneous and heterogeneous semi-solid pharmaceutical formulations. <i>International Journal of Pharmaceutics</i> , 2018, 552, 119-129.	2.6	22
59	Comparison of Principal Components Analysis, Independent Components Analysis and Common Components Analysis. <i>Journal of Analysis and Testing</i> , 2018, 2, 235-248.	2.5	27
60	ComDim for explorative multi-block data analysis of Cantal-type cheeses: Effects of salts, gentle heating and ripening. <i>Food Chemistry</i> , 2018, 264, 401-410.	4.2	11
61	Headspace solid-phase microextraction for wine volatile analysis. <i>Critical Reviews in Food Science and Nutrition</i> , 2017, 57, 2009-2020.	5.4	47
62	Analysis of time-resolved laser-induced breakdown spectra by mean field-independent components analysis (MFICA) and multivariate curve resolution-alternating least squares (MCR-ALS). <i>Journal of Chemometrics</i> , 2017, 31, e2869.	0.7	15
63	Multi-block data analysis using ComDim for the evaluation of complex samples: Characterization of edible oils. <i>Analytica Chimica Acta</i> , 2017, 961, 42-48.	2.6	23
64	An innovative chemometric method for processing direct introduction high resolution mass spectrometry metabolomic data: independent component discriminant analysis (ICDA). <i>Metabolomics</i> , 2017, 13, 1.	1.4	16
65	Synergetic Use of Principal Component Analysis Applied to Normed Physicochemical Measurements and GC-MS to Reveal the Stabilization Effect of Selected Essential Oils on Heated Rapeseed Oil. <i>Journal of Food Science</i> , 2017, 82, 1333-1343.	1.5	1
66	Solid-phase microextraction set-up for the analysis of liver volatolome to detect livestock exposure to micropollutants. <i>Journal of Chromatography A</i> , 2017, 1497, 9-18.	1.8	12
67	Contribution of fluorescence spectroscopy and independent components analysis to the evaluation of NaCl and KCl effects on molecular-structure and fat melting temperatures of Cantal-type cheese. <i>International Dairy Journal</i> , 2017, 73, 116-127.	1.5	17
68	Chemical Composition and Antimicrobial Activity of <i>Satureja</i> , <i>Thymus</i> , and <i>Thymbra</i> Species Grown in Lebanon. <i>Chemistry and Biodiversity</i> , 2017, 14, e1600236.	1.0	20
69	Combination of ¹ H NMR and chemometrics to discriminate manuka honey from other floral honey types from Oceania. <i>Food Chemistry</i> , 2017, 217, 766-772.	4.2	41
70	Detection of Blackcurrant Adulteration by Aronia Berry Using High Resolution Mass Spectrometry, Variable Selection and Combined PLS Regression Models. <i>Food Analytical Methods</i> , 2017, 10, 683-693.	1.3	3
71	Applications and challenges of multi-way calibration in electrochemical analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2017, 87, 32-48.	5.8	69
72	Analysis of target volatile compounds related to fishy off-flavor in heated rapeseed oil: A comparative study of different headspace techniques. <i>European Journal of Lipid Science and Technology</i> , 2016, 118, 906-918.	1.0	16

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73	Chemical Composition and Antimicrobial Activity of <i>Origanum libanoticum</i> , <i>Origanum ehrenbergii</i> , and <i>Origanum syriacum</i> Growing Wild in Lebanon. <i>Chemistry and Biodiversity</i> , 2016, 13, 555-560.	1.0	27
74	Investigation of fragrance stability used in the formulation of cosmetic and hygienic products using headspace solid-phase microextraction by nanostructured materials followed by gas chromatography with mass spectrometry. <i>Journal of Separation Science</i> , 2016, 39, 2760-2769.	1.3	4
75	Improved classification of fused data: Synergetic effect of partial least squares discriminant analysis (PLS-DA) and common components and specific weights analysis (CCSWA) combination as applied to tomato profiles (NMR, IR and IRMS). <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 156, 1-6.	1.8	27
76	Independent components analysis as a means to have initial estimates for multivariate curve resolution-alternating least squares. <i>Journal of Advanced Research</i> , 2016, 7, 795-802.	4.4	20
77	Data fusion between high resolution 1H-NMR and mass spectrometry: a synergetic approach to honey botanical origin characterization. <i>Analytical and Bioanalytical Chemistry</i> , 2016, 408, 4389-4401.	1.9	36
78	Independent Components Analysis. <i>Data Handling in Science and Technology</i> , 2016, 30, 225-277.	3.1	7
79	Analysis of multiblock datasets using ComDim: Overview and extension to the analysis of $(K + 1)$ datasets. <i>Journal of Chemometrics</i> , 2016, 30, 420-429.	0.7	38
80	Chemometric Tools to Highlight the Variability of the Chemical Composition and Yield of Lebanese <i>Origanum syriacum</i> L. Essential Oil. <i>Chemistry and Biodiversity</i> , 2016, 13, 1326-1347.	1.0	21
81	How to really perform high throughput metabolomic analyses efficiently?. <i>TrAC - Trends in Analytical Chemistry</i> , 2016, 85, 128-139.	5.8	27
82	Ascorbic acid and white wine production: a review of beneficial versus detrimental impacts. <i>Australian Journal of Grape and Wine Research</i> , 2016, 22, 169-181.	1.0	34
83	An overview of recent developments in volatile compounds analysis from edible oils: Technique-oriented perspectives. <i>European Journal of Lipid Science and Technology</i> , 2016, 118, 1853-1879.	1.0	31
84	Validation of a headspace trap gas chromatography and mass spectrometry method for the quantitative analysis of volatile compounds from degraded rapeseed oil. <i>Journal of Separation Science</i> , 2016, 39, 1675-1683.	1.3	12
85	Optimization of a liquid chromatography ion mobility-mass spectrometry method for untargeted metabolomics using experimental design and multivariate data analysis. <i>Analytica Chimica Acta</i> , 2016, 913, 55-62.	2.6	25
86	Use of the common components and specific weights analysis to interpret supersaturated designs. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 152, 97-106.	1.8	5
87	Characterization of surfactant complex mixtures using Raman spectroscopy and signal extraction methods: Application to laundry detergent reformulation. <i>Analytica Chimica Acta</i> , 2016, 915, 36-48.	2.6	9
88	Highlighting metabolic indicators of olive oil during storage by the AComDim method. <i>Food Chemistry</i> , 2016, 203, 104-116.	4.2	11
89	Interest of coupling ATR-MIR spectroscopy with independent components analysis to follow starch hydrothermal transformations. <i>Food Hydrocolloids</i> , 2016, 58, 298-307.	5.6	9
90	Using pH variations to improve the discrimination of wines by 3D front face fluorescence spectroscopy associated to Independent Components Analysis. <i>Talanta</i> , 2016, 153, 278-284.	2.9	34

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91	Common components and specific weights analysis: A tool for metabolomic data pre-processing. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 150, 41-50.	1.8	21
92	Attenuated total reflectance-mid infrared spectroscopy (ATR-MIR) coupled with independent components analysis (ICA): A fast method to determine plasticizers in polylactide (PLA). <i>Talanta</i> , 2016, 147, 569-580.	2.9	24
93	3D-front-face fluorescence spectroscopy and independent components analysis: A new way to monitor bread dough development. <i>Talanta</i> , 2016, 147, 307-314.	2.9	20
94	Application of independent components analysis with the JADE algorithm and NIR hyperspectral imaging for revealing food adulteration. <i>Journal of Food Engineering</i> , 2016, 168, 7-15.	2.7	61
95	PLS/OPLS models in metabolomics: the impact of permutation of dataset rows on the K-fold cross-validation quality parameters. <i>Molecular BioSystems</i> , 2015, 11, 13-19.	2.9	458
96	Comprehensive Two-dimensional Gas Chromatography for Analysis of the Volatile Compounds and Fishy Odor Off-flavors from Heated Rapeseed Oil. <i>Chromatographia</i> , 2015, 78, 805-817.	0.7	19
97	AComDim as a multivariate tool to analyse experimental design application to $\hat{1}^3$ -irradiated and leached ion exchange resins. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 141, 12-23.	1.8	9
98	Can we trust untargeted metabolomics? Results of the metabo-ring initiative, a large-scale, multi-instrument inter-laboratory study. <i>Metabolomics</i> , 2015, 11, 807-821.	1.4	112
99	DROP-D: Dimension reduction by orthogonal projection for discrimination. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 146, 221-231.	1.8	5
100	Independent components analysis to increase efficiency of discriminant analysis methods (FDA and Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.9	33
101	Fast and global authenticity screening of honey using $^1\text{H-NMR}$ profiling. <i>Food Chemistry</i> , 2015, 189, 60-66.	4.2	113
102	Spectrophotometric analysis of polysaccharide/milk protein interactions with methylene blue using Independent Components Analysis. <i>Food Hydrocolloids</i> , 2015, 43, 769-776.	5.6	17
103	Detection of orange juice frauds using front-face fluorescence spectroscopy and Independent Components Analysis. <i>Food Chemistry</i> , 2015, 168, 211-217.	4.2	51
104	3D front face solid-phase fluorescence spectroscopy combined with Independent Components Analysis to characterize organic matter in model soils. <i>Talanta</i> , 2014, 125, 146-152.	2.9	22
105	Optimizing separation conditions of 19 polycyclic aromatic hydrocarbons by cyclodextrin-modified capillary electrophoresis and applications to edible oils. <i>Talanta</i> , 2014, 119, 572-581.	2.9	27
106	Determination of rice type by $^1\text{H-NMR}$ spectroscopy in combination with different chemometric tools. <i>Journal of Chemometrics</i> , 2014, 28, 83-92.	0.7	46
107	Synergistic effect of the simultaneous chemometric analysis of $^1\text{H-NMR}$ spectroscopic and stable isotope (SNIF-NMR, ^{18}O , ^{13}C) data: Application to wine analysis. <i>Analytica Chimica Acta</i> , 2014, 833, 29-39.	2.6	81
108	An experimental design based strategy to optimize a capillary electrophoresis method for the separation of 19 polycyclic aromatic hydrocarbons. <i>Analytica Chimica Acta</i> , 2014, 820, 195-204.	2.6	14

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109	Application of independent component analysis on Raman images of a pharmaceutical drug product: Pure spectra determination and spatial distribution of constituents. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2014, 90, 78-84.	1.4	53
110	Rapid discrimination of plastic packaging materials using MIR spectroscopy coupled with independent components analysis (ICA). <i>Waste Management</i> , 2014, 34, 2131-2138.	3.7	65
111	Independent components analysis coupled with 3D-front-face fluorescence spectroscopy to study the interaction between plastic food packaging and olive oil. <i>Analytica Chimica Acta</i> , 2014, 839, 14-25.	2.6	28
112	Iterative weighting of multiblock data in the orthogonal partial least squares framework. <i>Analytica Chimica Acta</i> , 2014, 813, 25-34.	2.6	9
113	Human urinary biomarkers of dioxin exposure: Analysis by metabolomics and biologically driven data dimensionality reduction. <i>Toxicology Letters</i> , 2014, 230, 234-243.	0.4	51
114	Chemometric tools to highlight non-intentionally added substances (NIAS) in polyethylene terephthalate (PET). <i>Talanta</i> , 2013, 115, 928-937.	2.9	28
115	Independent components analysis applied to mid-infrared spectra of edible oils to study the thermal stability of heated oils. <i>Journal of Food Measurement and Characterization</i> , 2013, 7, 90-99.	1.6	9
116	Chemometric Tools to Highlight Possible Migration of Compounds from Packaging to Sunflower Oils. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 10565-10573.	2.4	11
117	Use of response surface methodology to optimize the simultaneous separation of eight polycyclic aromatic hydrocarbons by capillary zone electrophoresis with laser-induced fluorescence detection. <i>Journal of Chromatography A</i> , 2013, 1302, 181-190.	1.8	34
118	Development of a percutaneous penetration predictive model by SR-FTIR. <i>International Journal of Pharmaceutics</i> , 2013, 441, 628-635.	2.6	2
119	A consensus orthogonal partial least squares discriminant analysis (OPLS-DA) strategy for multiblock Omics data fusion. <i>Analytica Chimica Acta</i> , 2013, 769, 30-39.	2.6	246
120	Independent Components Analysis with the JADE algorithm. <i>TrAC - Trends in Analytical Chemistry</i> , 2013, 50, 22-32.	5.8	165
121	A multiway chemometric and kinetic study for evaluating the thermal stability of edible oils by ¹ H NMR analysis: Comparison of methods. <i>Talanta</i> , 2012, 88, 358-368.	2.9	29
122	Study of the heat stability of sunflower oil enriched in natural antioxidants by different analytical techniques and front-face fluorescence spectroscopy combined with Independent Components Analysis. <i>Talanta</i> , 2012, 99, 323-329.	2.9	28
123	The increase in oxidative stability of sunflower oil enriched with <i>Nigella sativa</i> L. Seed extracts. <i>Journal of Food Measurement and Characterization</i> , 2012, 6, 12-20.	1.6	4
124	Independent components analysis applied to 3D-front-face fluorescence spectra of edible oils to study the antioxidant effect of <i>Nigella sativa</i> L. extract on the thermal stability of heated oils. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 113, 32-42.	1.8	30
125	Application of 2D correlation spectroscopy on olive stones acid hydrolysates: Effect of overliming. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 113, 58-67.	1.8	13
126	Rare and Low Frequency Variant Stratification in the UK Population: Description and Impact on Association Tests. <i>PLoS ONE</i> , 2012, 7, e46519.	1.1	23

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127	A case study of extrapolation in NIR modelling – A chemometric challenge at –ChimioM@trie 2009–™. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 205-209.	1.8	7
128	Three-way principal component analysis applied to noodles sensory data analysis. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 125-130.	1.8	12
129	Examination of the potential for using chemical analysis as a surrogate for sensory analysis. Analytica Chimica Acta, 2010, 660, 2-7.	2.6	23
130	Development of near infrared sensors: Detection of influential factors by the AComDim method. Analytica Chimica Acta, 2010, 675, 16-23.	2.6	10
131	Preliminary studies on the mid-infrared analysis of edible oils by direct heating on an ATR diamond crystal. Food Chemistry, 2010, 120, 1170-1177.	4.2	36
132	Sensory, Chemical, and Electronic Tongue Assessment of Micro-oxygenated Wines and Oak Chip Maceration: Assessing the Commonality of Analytical Techniques. Journal of Agricultural and Food Chemistry, 2010, 58, 5026-5033.	2.4	26
133	Analytical methods for molecular gastronomy. Analytical and Bioanalytical Chemistry, 2009, 394, 659-661.	1.9	14
134	Combination of dynamic time warping and multivariate analysis for the comparison of comprehensive two-dimensional gas chromatograms. Journal of Chromatography A, 2009, 1216, 2866-2872.	1.8	64
135	Two new extensions of principal component transform to compute a PLS2 model between two wide matrices: PCT-PLS2 and segmented PCT-PLS2. Analytica Chimica Acta, 2009, 642, 37-44.	2.6	1
136	Improving the detection of significant factors using ANOVA-PCA by selective reduction of residual variability. Analytica Chimica Acta, 2009, 653, 131-142.	2.6	26
137	Fruit juice authentication by 1H NMR spectroscopy in combination with different chemometrics tools. Analytical and Bioanalytical Chemistry, 2008, 390, 419-427.	1.9	92
138	Using ANOVA-PCA for discriminant analysis: Application to the study of mid-infrared spectra of carraghenan gels as a function of concentration and temperature. Analytica Chimica Acta, 2008, 629, 47-55.	2.6	20
139	Multi-way analysis of outer product arrays using PARAFAC. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 170-178.	1.8	20
140	Segmented Principal Component Transform – Partial Least Squares regression. Chemometrics and Intelligent Laboratory Systems, 2007, 89, 59-68.	1.8	3
141	Selecting the optimum number of partial least squares components for the calibration of attenuated total reflectance-mid-infrared spectra of undesigned kerosene samples. Analytica Chimica Acta, 2007, 585, 253-265.	2.6	50
142	Independent component analysis as a pretreatment method for parallel factor analysis to eliminate artefacts from multiway data. Analytica Chimica Acta, 2007, 589, 216-224.	2.6	44
143	Evolving Window Zone Selection method followed by Independent Component Analysis as useful chemometric tools to discriminate between grapefruit juice, orange juice and blends. Analytica Chimica Acta, 2007, 597, 203-213.	2.6	28
144	Application of the ANOVA-PCA method to stability studies of reference materials. Analytica Chimica Acta, 2007, 603, 147-154.	2.6	21

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145	Non-invasive spectrophotometric sensing of carrot quality from harvest to consumption. <i>Postharvest Biology and Technology</i> , 2007, 45, 30-37.	2.9	45
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