## Douglas Neil Rutledge

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/303281/publications.pdf

Version: 2024-02-01

186 papers 5,615 citations

94381 37 h-index 64 g-index

193 all docs

193 docs citations

times ranked

193

6559 citing authors

| #  | Article   | IF           | CITATIONS |
|----|---|--------------|-----------|
| 1  | PLS/OPLS models in metabolomics: the impact of permutation of dataset rows on the K-fold cross-validation quality parameters. Molecular BioSystems, 2015, 11, 13-19.                                      | 2.9          | 458       |
| 2  | A consensus orthogonal partial least squares discriminant analysis (OPLS-DA) strategy for multiblock Omics data fusion. Analytica Chimica Acta, 2013, 769, 30-39.   | 2.6          | 246       |
| 3  | Multivariate analysis of uronic acid and neutral sugars in whole pectic samples by FT-IR spectroscopy.<br>Carbohydrate Polymers, 1998, 37, 241-248.   | 5.1          | 179       |
| 4  | New data preprocessing trends based on ensemble of multiple preprocessing techniques. TrAC - Trends in Analytical Chemistry, 2020, 132, 116045.   | 5.8          | 173       |
| 5  | Independent Components Analysis with the JADE algorithm. TrAC - Trends in Analytical Chemistry, 2013, 50, 22-32.  | 5 <b>.</b> 8 | 165       |
| 6  | FTIR spectroscopy as a tool for the analysis of olive pulp cell-wall polysaccharide extracts. Carbohydrate Research, 1999, 317, 145-154.  | 1.1          | 141       |
| 7  | Assessment of protein glycation markers in infant formulas. Food Chemistry, 2004, 87, 253-259.  | 4.2          | 122       |
| 8  | Fast and global authenticity screening of honey using 1H-NMR profiling. Food Chemistry, 2015, 189, 60-66.   | 4.2          | 113       |
| 9  | Can we trust untargeted metabolomics? Results of the metabo-ring initiative, a large-scale, multi-instrument inter-laboratory study. Metabolomics, 2015, 11, 807-821.                                     | 1.4          | 112       |
| 10 | Fruit juice authentication by 1H NMR spectroscopy in combination with different chemometrics tools. Analytical and Bioanalytical Chemistry, 2008, 390, 419-427.   | 1.9          | 92        |
| 11 | Robustness of models developed by multivariate calibration. Part I. TrAC - Trends in Analytical Chemistry, 2004, 23, 157-170.   | 5 <b>.</b> 8 | 91        |
| 12 | Fluorescence spectroscopy for monitoring deterioration of extra virgin olive oil during heating. Analytical and Bioanalytical Chemistry, 2005, 382, 1438-1443.  | 1.9          | 90        |
| 13 | Recent trends in multi-block data analysis in chemometrics for multi-source data integration. TrAC - Trends in Analytical Chemistry, 2021, 137, 116206.   | 5.8          | 86        |
| 14 | Synergistic effect of the simultaneous chemometric analysis of 1H NMR spectroscopic and stable isotope (SNIF-NMR, 18O, 13C) data: Application to wine analysis. Analytica Chimica Acta, 2014, 833, 29-39. | 2.6          | 81        |
| 15 | Determination of the degree of methylesterification of pectic polysaccharides by FT-IR using an outer product PLS1 regression. Carbohydrate Polymers, 2002, 50, 85-94.                                    | 5.1          | 79        |
| 16 | Applications and challenges of multi-way calibration inÂelectrochemical analysis. TrAC - Trends in Analytical Chemistry, 2017, 87, 32-48.   | 5.8          | 69        |
| 17 | Durbin–Watson statistic as a morphological estimator of information content. Analytica Chimica Acta, 2002, 454, 277-295.  | 2.6          | 65        |
| 18 | Rapid discrimination of plastic packaging materials using MIR spectroscopy coupled with independent components analysis (ICA). Waste Management, 2014, 34, 2131-2138.                                     | 3.7          | 65        |

| #  | Article  | IF  | Citations |
|----|--|-----|-----------|
| 19 | 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        |
| 20 | Application of independent components analysis with the JADE algorithm and NIR hyperspectral imaging for revealing food adulteration. Journal of Food Engineering, 2016, 168, 7-15.  | 2.7 | 61        |
| 21 | Application of independent component analysis on Raman images of a pharmaceutical drug product: Pure spectra determination and spatial distribution of constituents. Journal of Pharmaceutical and Biomedical Analysis, 2014, 90, 78-84. | 1.4 | 53        |
| 22 | Chemometric pre-processing can negatively affect the performance of near-infrared spectroscopy models for fruit quality prediction. Talanta, 2021, 229, 122303.  | 2.9 | 53        |
| 23 | Application of support vector machines to 1H NMR data of fish oils: methodology for the confirmation of wild and farmed salmon and their origins. Analytical and Bioanalytical Chemistry, 2007, 387, 1499-1510.                          | 1.9 | 52        |
| 24 | Human urinary biomarkers of dioxin exposure: Analysis by metabolomics and biologically driven data dimensionality reduction. Toxicology Letters, 2014, 230, 234-243.   | 0.4 | 51        |
| 25 | Detection of orange juice frauds using front-face fluorescence spectroscopy and Independent Components Analysis. Food Chemistry, 2015, 168, 211-217.   | 4.2 | 51        |
| 26 | 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        |
| 27 | MATLAB in electrochemistry: A review. Talanta, 2019, 194, 205-225.   | 2.9 | 50        |
| 28 | SPORT pre-processing can improve near-infrared quality prediction models for fresh fruits and agro-materials. Postharvest Biology and Technology, 2020, 168, 111271.   | 2.9 | 48        |
| 29 | Headspace solid-phase microextraction for wine volatile analysis. Critical Reviews in Food Science and Nutrition, 2017, 57, 2009-2020.   | 5.4 | 47        |
| 30 | An NMR Relaxation Study of the State of Water in Gelatin Gels. Journal of Magnetic Resonance, 1999, 138, 36-42.  | 1.2 | 46        |
| 31 | Determination of rice type by <sup>1</sup> H NMR spectroscopy in combination with different chemometric tools. Journal of Chemometrics, 2014, 28, 83-92.   | 0.7 | 46        |
| 32 | Non-invasive spectrophotometric sensing of carrot quality from harvest to consumption. Postharvest Biology and Technology, 2007, 45, 30-37.  | 2.9 | 45        |
| 33 | Multivariate statistical analysis of two-dimensional NMR data to differentiate grapevine cultivars and clones. Food Chemistry, 1996, 57, 441-450.  | 4.2 | 44        |
| 34 | 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        |
| 35 | Combination of 1H NMR and chemometrics to discriminate manuka honey from other floral honey types from Oceania. Food Chemistry, 2017, 217, 766-772.  | 4.2 | 41        |
| 36 | Relations between Mid-Infrared and Near-Infrared Spectra Detected by Analysis of Variance of an Intervariable Data Matrix. Applied Spectroscopy, 1997, 51, 1384-1393.  | 1.2 | 39        |

| #  | Article   | IF         | Citations     |
|----|---|------------|---------------|
| 37 | Are standard sample measurements still needed to transfer multivariate calibration models between near-infrared spectrometers? The answer is not always. TrAC - Trends in Analytical Chemistry, 2021, 143, 116331.  | 5.8        | 39            |
| 38 | Multivariate statistical analysis of gas chromatograms to differentiate cocoa masses by geographical origin and roasting conditions. Analyst, The, 1994, 119, 1171-1176.  | 1.7        | 38            |
| 39 | Analysis of multiblock datasets using ComDim: Overview and extension to the analysis of ( <i>K</i> + 1) datasets. Journal of Chemometrics, 2016, 30, 420-429.   | 0.7        | 38            |
| 40 | Outer-product analysis (OPA) using PCA to study the influence of temperature on NIR spectra of water. Vibrational Spectroscopy, 2005, 39, 50-58.  | 1.2        | 37            |
| 41 | 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            |
| 42 | Data fusion between high resolution 1H-NMR and mass spectrometry: a synergetic approach to honey botanical origin characterization. Analytical and Bioanalytical Chemistry, 2016, 408, 4389-4401.   | 1.9        | 36            |
| 43 | MBA-GUI: A chemometric graphical user interface for multi-block data visualisation, regression, classification, variable selection and automated pre-processing. Chemometrics and Intelligent Laboratory Systems, 2020, 205, 104139.                                  | 1.8        | 36            |
| 44 | Two standard-free approaches to correct for external influences on near-infrared spectra to make models widely applicable. Postharvest Biology and Technology, 2020, 170, 111326.   | 2.9        | 36            |
| 45 | Discrimination of wines based on 2D NMR spectra using learning vector quantization neural networks and partial least squares discriminant analysis. Analytica Chimica Acta, 2006, 558, 144-149.   | 2.6        | 35            |
| 46 | Comparison of common components analysis with principal components analysis and independent components analysis: Application to SPME-GC-MS volatolomic signatures. Talanta, 2018, 178, 854-863.   | 2.9        | 35            |
| 47 | Use of response surface methodology to optimize the simultaneous separation of eight polycyclic aromatic hydrocarbons by capillary zone electrophoresis with laser-induced fluorescence detection. Journal of Chromatography A, 2013, 1302, 181-190.                  | 1.8        | 34            |
| 48 | Ascorbic acid and white wine production: a review of beneficial versus detrimental impacts. Australian Journal of Grape and Wine Research, 2016, 22, 169-181.   | 1.0        | 34            |
| 49 | Using pH variations to improve the discrimination of wines by 3D front face fluorescence spectroscopy associated to Independent Components Analysis. Talanta, 2016, 153, 278-284.   | 2.9        | 34            |
| 50 | Independent components analysis to increase efficiency of discriminant analysis methods (FDA and) Tj ETQq0 0  | 0 rgBT /Ov | verlock 10 Tf |
| 51 | An overview of recent developments in volatile compounds analysis from edible oils:<br>Techniqueâ€oriented perspectives. European Journal of Lipid Science and Technology, 2016, 118, 1853-1879.  | 1.0        | 31            |
| 52 | Monitoring Freeze-Drying by Low Resolution Pulse NMR: Determination of Sublimation Endpoint. Journal of Food Science, 1991, 56, 1707-1710.  | 1.5        | 30            |
| 53 | Independent components analysis applied to 3D-front-face fluorescence spectra of edible oils to study the antioxidant effect of Nigella sativa L. extract on the thermal stability of heated oils. Chemometrics and Intelligent Laboratory Systems, 2012, 113, 32-42. | 1.8        | 30            |
| 54 | A multiway chemometric and kinetic study for evaluating the thermal stability of edible oils by 1H NMR analysis: Comparison of methods. Talanta, 2012, 88, 358-368.   | 2.9        | 29            |

| #  | Article   | IF  | CITATIONS |
|----|---|-----|-----------|
| 55 | 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        |
| 56 | 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. Talanta, 2012, 99, 323-329.  | 2.9 | 28        |
| 57 | Chemometric tools to highlight non-intentionally added substances (NIAS) in polyethylene terephthalate (PET). Talanta, 2013, 115, 928-937.  | 2.9 | 28        |
| 58 | Independent components analysis coupled with 3D-front-face fluorescence spectroscopy to study the interaction between plastic food packaging and olive oil. Analytica Chimica Acta, 2014, 839, 14-25.   | 2.6 | 28        |
| 59 | Optimizing separation conditions of 19 polycyclic aromatic hydrocarbons by cyclodextrin-modified capillary electrophoresis and applications to edible oils. Talanta, 2014, 119, 572-581.  | 2.9 | 27        |
| 60 | Chemical Composition and Antimicrobial Activity of <i>Origanum libanoticum</i> , <i>Origanum ehrenbergii</i> , and <i>Origanum syriacum</i> Growing Wild in Lebanon. Chemistry and Biodiversity, 2016, 13, 555-560.   | 1.0 | 27        |
| 61 | 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). Chemometrics and Intelligent Laboratory Systems, 2016, 156, 1-6. | 1.8 | 27        |
| 62 | How to really perform high throughput metabolomic analyses efficiently?. TrAC - Trends in Analytical Chemistry, 2016, 85, 128-139.  | 5.8 | 27        |
| 63 | ComDim: From multiblock data analysis to path modeling. Food Quality and Preference, 2018, 67, 27-34.   | 2.3 | 27        |
| 64 | Comparison of Principal Components Analysis, Independent Components Analysis and Common Components Analysis. Journal of Analysis and Testing, 2018, 2, 235-248.   | 2.5 | 27        |
| 65 | Automatic de-noising of close-range hyperspectral images with a wavelength-specific shearlet-based image noise reduction method. Sensors and Actuators B: Chemical, 2019, 281, 1034-1044.   | 4.0 | 27        |
| 66 | 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        |
| 67 | Sensory, Chemical, and Electronic Tongue Assessment of Micro-oxygenated Wines and Oak Chip<br>Maceration: Assessing the Commonality of Analytical Techniques. Journal of Agricultural and Food<br>Chemistry, 2010, 58, 5026-5033.   | 2.4 | 26        |
| 68 | MAGNETIC RESONANCE IMAGING STUDIES of the FREEZE-DRYING KINETICS of POTATO. Journal of Food Process Engineering, 1994, 17, 325-352.   | 1.5 | 25        |
| 69 | Optimization of a liquid chromatography ion mobility-mass spectrometry method for untargeted metabolomics using experimental design and multivariate data analysis. Analytica Chimica Acta, 2016, 913, 55-62.   | 2.6 | 25        |
| 70 | Determination of the optimal number of components in independent components analysis. Talanta, 2018, 179, 538-545.  | 2.9 | 25        |
| 71 | Independent components analysis (ICA) at the "cocktail-party―in analytical chemistry. Talanta, 2020, 208, 120451.   | 2.9 | 25        |
| 72 | Hydration Properties and the Role of Water in Taste Modalities of Sucrose, Caffeine, and Sucroseâ^Caffeine Mixtures. Journal of Agricultural and Food Chemistry, 2001, 49, 4039-4045.   | 2.4 | 24        |

| #  | Article   | IF  | CITATIONS |
|----|---|-----|-----------|
| 73 | Attenuated total reflectance-mid infrared spectroscopy (ATR-MIR) coupled with independent components analysis (ICA): A fast method to determine plasticizers in polylactide (PLA). Talanta, 2016, 147, 569-580.                                 | 2.9 | 24        |
| 74 | Examination of the potential for using chemical analysis as a surrogate for sensory analysis. Analytica Chimica Acta, 2010, 660, 2-7.   | 2.6 | 23        |
| 75 | Multi-block data analysis using ComDim for the evaluation of complex samples: Characterization of edible oils. Analytica Chimica Acta, 2017, 961, 42-48.  | 2.6 | 23        |
| 76 | Rare and Low Frequency Variant Stratification in the UK Population: Description and Impact on Association Tests. PLoS ONE, 2012, 7, e46519.   | 1.1 | 23        |
| 77 | PoLiSh — smoothed partial least-squares regression. Analytica Chimica Acta, 2001, 446, 279-294.   | 2.6 | 22        |
| 78 | Principal components transform-partial least squares: a novel method to accelerate cross-validation in PLS regression. Chemometrics and Intelligent Laboratory Systems, 2004, 73, 245-255.  | 1.8 | 22        |
| 79 | 3D front face solid-phase fluorescence spectroscopy combined with Independent Components Analysis to characterize organic matter in model soils. Talanta, 2014, 125, 146-152.   | 2.9 | 22        |
| 80 | Comparison of different chemometric methods to extract chemical and physical information from Raman images of homogeneous and heterogeneous semi-solid pharmaceutical formulations. International Journal of Pharmaceutics, 2018, 552, 119-129. | 2.6 | 22        |
| 81 | Urinary Metabolomics Profiles Associated to Bovine Meat Ingestion in Humans. Molecular Nutrition and Food Research, 2019, 63, e1700834.   | 1.5 | 22        |
| 82 | Application of the ANOVA-PCA method to stability studies of reference materials. Analytica Chimica Acta, 2007, 603, 147-154.  | 2.6 | 21        |
| 83 | Chemometric Tools to Highlight the Variability of the Chemical Composition and Yield of Lebanese <i>Origanum syriacum </i> L. Essential Oil. Chemistry and Biodiversity, 2016, 13, 1326-1347.   | 1.0 | 21        |
| 84 | Common components and specific weights analysis: A tool for metabolomic data pre-processing. Chemometrics and Intelligent Laboratory Systems, 2016, 150, 41-50.   | 1.8 | 21        |
| 85 | Parallel pre-processing through orthogonalization (PORTO) and its application to near-infrared spectroscopy. Chemometrics and Intelligent Laboratory Systems, 2021, 212, 104190.  | 1.8 | 21        |
| 86 | Multi-way analysis of outer product arrays using PARAFAC. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 170-178.   | 1.8 | 20        |
| 87 | 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        |
| 88 | Independent components analysis as a means to have initial estimates for multivariate curve resolution-alternating least squares. Journal of Advanced Research, 2016, 7, 795-802.   | 4.4 | 20        |
| 89 | 3D-front-face fluorescence spectroscopy and independent components analysis: A new way to monitor bread dough development. Talanta, 2016, 147, 307-314.   | 2.9 | 20        |
| 90 | Chemical Composition and Antimicrobial Activity of <i>Satureja</i> Thymbra Species Grown in Lebanon. Chemistry and Biodiversity, 2017, 14, e1600236.  | 1.0 | 20        |

| #   | Article  | IF  | Citations |
|-----|--|-----|-----------|
| 91  | Comprehensive Two-dimensional Gas Chromatography for Analysis of the Volatile Compounds and Fishy Odor Off-flavors from Heated Rapeseed Oil. Chromatographia, 2015, 78, 805-817.   | 0.7 | 19        |
| 92  | Characterisation of water in agro-food products by time domain-NMR. Food Control, 2001, 12, 437-445.   | 2.8 | 18        |
| 93  | Detection of Heterogeneous Wheat Samples Using near Infrared Spectroscopy. Journal of Near Infrared Spectroscopy, 2003, 11, 109-121.   | 0.8 | 18        |
| 94  | A variable selection method for multiclass classification problems using two-class ROC analysis. Chemometrics and Intelligent Laboratory Systems, 2018, 177, 35-46.  | 1.8 | 18        |
| 95  | Assessment of the microbial interplay during anaerobic co-digestion of wastewater sludge using common components analysis. PLoS ONE, 2020, 15, e0232324.   | 1.1 | 18        |
| 96  | Segmented principal component transform–principal component analysis. Chemometrics and Intelligent Laboratory Systems, 2005, 78, 125-137.  | 1.8 | 17        |
| 97  | Outer-product analysis (OPA) using PLS regression to study the retrogradation of starch. Vibrational Spectroscopy, 2006, 40, 10-19.  | 1.2 | 17        |
| 98  | Spectrophotometric analysis of polysaccharide/milk protein interactions with methylene blue using Independent Components Analysis. Food Hydrocolloids, 2015, 43, 769-776.  | 5.6 | 17        |
| 99  | 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. International Dairy Journal, 2017, 73, 116-127.             | 1.5 | 17        |
| 100 | ComDim Methods for the Analysis of Multiblock Data in aÂData Fusion Perspective. Data Handling in Science and Technology, 2019, , 179-204.   | 3.1 | 17        |
| 101 | Evaluation of an untargeted chemometric approach for the source inference of ignitable liquids in forensic science. Forensic Science International, 2019, 295, 8-18.   | 1.3 | 17        |
| 102 | Utilising variable sorting for normalisation to correct illumination effects in close-range spectral images of potato plants. Biosystems Engineering, 2020, 197, 318-323.  | 1.9 | 17        |
| 103 | Application of 2D correlation spectroscopy and outer product analysis to infrared spectra of sugar beets. Vibrational Spectroscopy, 2004, 36, 279-285.   | 1.2 | 16        |
| 104 | Analysis of target volatile compounds related to fishy offâ€flavor in heated rapeseed oil: A comparative study of different headspace techniques. European Journal of Lipid Science and Technology, 2016, 118, 906-918.  | 1.0 | 16        |
| 105 | An innovative chemometric method for processing direct introduction high resolution mass spectrometry metabolomic data: independent componentâ $\in$ discriminant analysis (ICâ $\in$ DA). Metabolomics, 2017, 13, 1.  | 1.4 | 16        |
| 106 | Analysis of timeâ€resolved laserâ€induced breakdown spectra by mean fieldâ€independent components analysis ( <scp>MFICA</scp> ) and multivariate curve resolution–alternating least squares ( <scp>MCRâ€ALS</scp> ). Journal of Chemometrics, 2017, 31, e2869. | 0.7 | 15        |
| 107 | Complementary chemometrics and deep learning for semantic segmentation of tall and wide visible and near-infrared spectral images of plants. Computers and Electronics in Agriculture, 2021, 186, 106226.  | 3.7 | 15        |
| 108 | Analytical methods for molecular gastronomy. Analytical and Bioanalytical Chemistry, 2009, 394, 659-661.   | 1.9 | 14        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 109 | An experimental design based strategy to optimize a capillary electrophoresis method for the separation of 19 polycyclic aromatic hydrocarbons. Analytica Chimica Acta, 2014, 820, 195-204.   | 2.6 | 14        |
| 110 | Fluorescence spectroscopy coupled with independent components analysis to monitor molecular changes during heating and cooling of Cantalâ€type cheeses with different NaCl and KCl contents. Journal of the Science of Food and Agriculture, 2018, 98, 963-975.               | 1.7 | 14        |
| 111 | Application of 2D correlation spectroscopy on olive stones acid hydrolysates: Effect of overliming. Chemometrics and Intelligent Laboratory Systems, 2012, 113, 58-67.  | 1.8 | 13        |
| 112 | An untargeted evaluation of food contact materials by flow injection analysis-mass spectrometry (FIA-MS) combined with independent components analysis (ICA). Analytica Chimica Acta, 2018, 1022, 81-88.  | 2.6 | 13        |
| 113 | Changes in Red Wine Composition during Bottle Aging: Impacts of Grape Variety, Vineyard Location, Maturity, and Oxygen Availability during Aging. Journal of Agricultural and Food Chemistry, 2020, 68, 13331-13343.  | 2.4 | 13        |
| 114 | Three-way principal component analysis applied to noodles sensory data analysis. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 125-130.   | 1.8 | 12        |
| 115 | Validation of a headspace trap gas chromatography and mass spectrometry method for the quantitative analysis of volatile compounds from degraded rapeseed oil. Journal of Separation Science, 2016, 39, 1675-1683.  | 1.3 | 12        |
| 116 | Solid-phase microextraction set-up for the analysis of liver volatolome to detect livestock exposure to micropollutants. Journal of Chromatography A, 2017, 1497, 9-18.   | 1.8 | 12        |
| 117 | Characterisation of cocoa masses: low resolution pulse NMR study of the effect of geographical origin and roasting on fluidification. Food Chemistry, 1994, 49, 83-93.  | 4.2 | 11        |
| 118 | Chemometric Tools to Highlight Possible Migration of Compounds from Packaging to Sunflower Oils. Journal of Agricultural and Food Chemistry, 2013, 61, 10565-10573.   | 2.4 | 11        |
| 119 | Highlighting metabolic indicators of olive oil during storage by the AComDim method. Food Chemistry, 2016, 203, 104-116.  | 4.2 | 11        |
| 120 | ComDim for explorative multi-block data analysis of Cantal-type cheeses: Effects of salts, gentle heating and ripening. Food Chemistry, 2018, 264, 401-410.   | 4.2 | 11        |
| 121 | Assessment of substrate biodegradability improvement in anaerobic Co-digestion using a chemometrics-based metabolomic approach. Chemosphere, 2020, 254, 126812.   | 4.2 | 11        |
| 122 | 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. Chemometrics and Intelligent Laboratory Systems, 2022, 222, 104497. | 1.8 | 11        |
| 123 | Method for detecting information in signals: application to two-dimensional time domain NMR dataâ€. Analyst, The, 1998, 123, 551-559.   | 1.7 | 10        |
| 124 | Correction of biased time domain NMR estimates of the solid content of partially crystallized systems. Applied Magnetic Resonance, 2002, 22, 335-346.   | 0.6 | 10        |
| 125 | Homogeneity check of agricultural and food industries samples using near infrared spectroscopy.<br>Analytical and Bioanalytical Chemistry, 2003, 375, 496-504.  | 1.9 | 10        |
| 126 | Development of near infrared sensors: Detection of influential factors by the AComDim method. Analytica Chimica Acta, 2010, 675, 16-23.   | 2.6 | 10        |

| #   | Article  | IF  | Citations |
|-----|--|-----|-----------|
| 127 | Effect of ammonia exposure and acclimation on the performance and the microbiome of anaerobic digestion. Bioresource Technology Reports, 2020, 11, 100488.   | 1.5 | 10        |
| 128 | Discriminability and uncertainty in principal component analysis (PCA) of temporal check-all-that-apply (TCATA) data. Food Quality and Preference, 2022, 96, 104370.   | 2.3 | 10        |
| 129 | Metataxonomics, metagenomics and metabolomics analysis of the influence of temperature modification in full-scale anaerobic digesters. Bioresource Technology, 2022, 346, 126612.  | 4.8 | 10        |
| 130 | Independent components analysis applied to mid-infrared spectra of edible oils to study the thermal stability of heated oils. Journal of Food Measurement and Characterization, 2013, 7, 90-99.  | 1.6 | 9         |
| 131 | Iterative weighting of multiblock data in the orthogonal partial least squares framework. Analytica Chimica Acta, 2014, 813, 25-34.  | 2.6 | 9         |
| 132 | AComDim as a multivariate tool to analyse experimental design application to $\hat{1}^3$ -irradiated and leached ion exchange resins. Chemometrics and Intelligent Laboratory Systems, 2015, 141, 12-23.   | 1.8 | 9         |
| 133 | Characterization of surfactant complex mixtures using Raman spectroscopy and signal extraction methods: Application to laundry detergent deformulation. Analytica Chimica Acta, 2016, 915, 36-48.  | 2.6 | 9         |
| 134 | Interest of coupling ATR-MIR spectroscopy with independent components analysis to follow starch hydrothermal transformations. Food Hydrocolloids, 2016, 58, 298-307.   | 5.6 | 9         |
| 135 | A generic workflow combining deep learning and chemometrics for processing close-range spectral images to detect drought stress in Arabidopsis thaliana to support digital phenotyping. Chemometrics and Intelligent Laboratory Systems, 2021, 216, 104373.                                  | 1.8 | 9         |
| 136 | Exploratory study on the possibility to link gasoline samples sharing a common source after alteration by evaporation or combustion. Forensic Science International, 2019, 301, 190-201.   | 1.3 | 8         |
| 137 | Chemical Variability of the Essential Oil of Origanum ehrenbergii Boiss. from Lebanon, Assessed by Independent Component Analysis (ICA) and Common Component and Specific Weight Analysis (CCSWA). International Journal of Molecular Sciences, 2019, 20, 1026.                              | 1.8 | 8         |
| 138 | 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. European Journal of Mass Spectrometry, 2019, 25, 251-258. | 0.5 | 8         |
| 139 | FRUITNIR-GUI: A graphical user interface for correcting external influences in multi-batch near infrared experiments related to fruit quality prediction. Postharvest Biology and Technology, 2021, 175, 111414.   | 2.9 | 8         |
| 140 | Is the Calibration Transfer of Multivariate Calibration Models between High- and Low-Field NMR Instruments Possible? A Case Study of Lignin Molecular Weight. Analytical Chemistry, 2022, 94, 3997-4004.   | 3.2 | 8         |
| 141 | A case study of extrapolation in NIR modelling — A chemometric challenge at â€ <sup>*</sup> Chimiométrie 2009'.<br>Chemometrics and Intelligent Laboratory Systems, 2011, 106, 205-209.  | 1.8 | 7         |
| 142 | Independent Components Analysis. Data Handling in Science and Technology, 2016, 30, 225-277.   | 3.1 | 7         |
| 143 | A short note on achieving similar performance to deep learning with practical chemometrics. Chemometrics and Intelligent Laboratory Systems, 2021, 214, 104336.  | 1.8 | 7         |
| 144 | Different Methods for Determining the Dimensionality of Multivariate Models. Frontiers in Analytical Science, 2021, 1, .   | 1.1 | 7         |

| #   | Article   | IF  | Citations |
|-----|---|-----|-----------|
| 145 | Analysis of the ozonation products of phthalic acid in water using combined high-performance liquid chromatography-mass spectrometry. Analyst, The, 1984, 109, 817.   | 1.7 | 6         |
| 146 | Biological reference materials for the verification of sample preparation and measurement by low resolution NMR. Fresenius' Journal of Analytical Chemistry, 1990, 338, 441-448.  | 1.5 | 6         |
| 147 | Potential of dynamically harmonized Fourier transform ion cyclotron resonance cell for high-throughput metabolomics fingerprinting: control of data quality. Analytical and Bioanalytical Chemistry, 2018, 410, 483-490.  | 1.9 | 6         |
| 148 | Evaluation of the impact of buffered peptone water composition on the discrimination between Salmonella enterica and Escherichia coli by Raman spectroscopy. Analytical and Bioanalytical Chemistry, 2020, 412, 3595-3604.  | 1.9 | 6         |
| 149 | Chapter 9 A windows program for relaxation parameter estimation. Data Handling in Science and Technology, 1996, , 191-217.  | 3.1 | 5         |
| 150 | Hydration state of gelatine studied by time domain nuclear magnetic resonance (TD-NMR): a preliminary study. Food Chemistry, 1996, 57, 287-293.   | 4.2 | 5         |
| 151 | DROP-D: Dimension reduction by orthogonal projection for discrimination. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 221-231.   | 1.8 | 5         |
| 152 | Use of the common components and specific weights analysis to interpret supersaturated designs. Chemometrics and Intelligent Laboratory Systems, 2016, 152, 97-106.   | 1.8 | 5         |
| 153 | Extraction of information about structural changes in a semisolid pharmaceutical formulation from nearâ€infrared and Raman images by multivariate curve resolution–alternating least squares and ComDim. Journal of Chemometrics, 2020, 34, e3288.                                | 0.7 | 5         |
| 154 | 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. Nutrients, 2021, 13, 1191.                                     | 1.7 | 5         |
| 155 | The increase in oxidative stability of sunflower oil enriched with Nigella sativa L. Seed extracts. Journal of Food Measurement and Characterization, 2012, 6, 12-20.   | 1.6 | 4         |
| 156 | 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. Journal of Separation Science, 2016, 39, 2760-2769. | 1.3 | 4         |
| 157 | Multiblock modelling on the study of the kinetic degradation of rosuvastatin calcium in the presence of retention time shifts and rank deficiency. Analytica Chimica Acta, 2020, 1133, 77-87.   | 2.6 | 4         |
| 158 | Pre-processing Methods. , 2020, , 1-75.   |     | 4         |
| 159 | Monte Carlo methods for estimating Mallows's Cp and AIC criteria for PLSR models. Illustration on agronomic spectroscopic NIR data. Journal of Chemometrics, 2021, 35, e3369.   | 0.7 | 4         |
| 160 | Digital images and independent components analysis in the determination of bioactive compounds from grape juice. LWT - Food Science and Technology, 2021, 152, 112308.  | 2.5 | 4         |
| 161 | Monitoring hydrogenation in the margarine industry by low resolution pulsed NMR. Journal of the Science of Food and Agriculture, 1990, 53, 389-393.   | 1.7 | 3         |
| 162 | Proficiency testing schemes: solutions for homogeneity control. Accreditation and Quality Assurance, 2004, 9, 333-339.  | 0.4 | 3         |

| #   | Article   | IF  | Citations |
|-----|---|-----|-----------|
| 163 | Segmented Principal Component Transform–Partial Least Squares regression. Chemometrics and Intelligent Laboratory Systems, 2007, 89, 59-68.   | 1.8 | 3         |
| 164 | Generalised PLS_Cluster: an extension of PLS_Cluster for interpretable hierarchical clustering of multivariate data. Sensing and Instrumentation for Food Quality and Safety, 2007, 1, 79-90.   | 1.5 | 3         |
| 165 | Detection of Blackcurrant Adulteration by Aronia Berry Using High Resolution Mass Spectrometry,<br>Variable Selection and Combined PLS Regression Models. Food Analytical Methods, 2017, 10, 683-693.   | 1.3 | 3         |
| 166 | Investigation of Origanum libanoticum Essential Oils Chemical Polymorphism by Independent Components Analysis (ICA). Natural Product Communications, 2018, 13, 1934578X1801301.   | 0.2 | 3         |
| 167 | Raman Imaging and Chemometrics Evaluation of Natural and Synthetic Beeswaxes as Matrices for Nanostructured Lipid Carriers Development. Brazilian Journal of Analytical Chemistry, 2021, 8, .   | 0.3 | 3         |
| 168 | Rearrangement of incomplete multi-omics datasets combined with ComDim for evaluating replicate cross-platform variability and batch influence. Chemometrics and Intelligent Laboratory Systems, 2021, 218, 104422.                                | 1.8 | 3         |
| 169 | Response oriented covariates selection (ROCS) for fast block order- and scale-independent variable selection in multi-block scenarios. Chemometrics and Intelligent Laboratory Systems, 2022, , 104551.   | 1.8 | 3         |
| 170 | Development of a percutaneous penetration predictive model by SR-FTIR. International Journal of Pharmaceutics, 2013, 441, 628-635.  | 2.6 | 2         |
| 171 | A Proposed Implementation of JCAMP-DX. NIR News, 1991, 2, 6-7.  | 1.6 | 2         |
| 172 | A tutorial on the analysis of multifactorial designs from one or more data sources using AComDim. Journal of Chemometrics, 2023, 37, .  | 0.7 | 2         |
| 173 | Exogenous application of bioregulators in Coffea arabica beans during ripening: Investigation of UVâ€"Visible and NIR mixture design-fingerprints using AComDim-ICA. Microchemical Journal, 2022, 181, 107702.                                    | 2.3 | 2         |
| 174 | The international spectroscopic data bank "EuroSpecâ€, a new way of exchange within the scientific community. Vibrational Spectroscopy, 2004, 36, 191-193.  | 1.2 | 1         |
| 175 | Polar coordinates projection: A simple data visualization tool. TrAC - Trends in Analytical Chemistry, 2005, 24, 839-842.   | 5.8 | 1         |
| 176 | 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         |
| 177 | Synergetic Use of Principal Component Analysis Applied to Normed Physicochemical Measurements and GC × GCâ€MS to Reveal the Stabilization Effect of Selected Essential Oils on Heated Rapeseed Oil. Journal of Food Science, 2017, 82, 1333-1343. | 1.5 | 1         |
| 178 | Quantification of palm oil bioactive compounds by ultraâ€highâ€performance supercritical fluid chromatography and chemometrics. Canadian Journal of Chemical Engineering, 2021, , .   | 0.9 | 1         |
| 179 | Stability study of furans, glucose and xylose under overliming conditions: Effect of sugar degradation products. Bioresource Technology Reports, 2021, 15, 100722.  | 1.5 | 1         |
| 180 | Modelling of statistical tables for outlier tests. Chemometrics and Intelligent Laboratory Systems, 1990, 9, 257-259.   | 1.8 | 0         |

| #   | Article  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 181 | Factorial correspondence regression applied to multi-way spectral data. Analyst, The, 1998, 123, 1783-1790.  | 1.7 | O         |
| 182 | In vino analytica scientia 2003. Analytica Chimica Acta, 2004, 513, 1.   | 2.6 | O         |
| 183 | Molecular Markers of Dietary Essential Amino Acid-deficiency (P08-059-19). Current Developments in Nutrition, 2019, 3, nzz044.P08-059-19.  | 0.1 | O         |
| 184 | Molecular markers of dietary essential amino acid-deficiency. Proceedings of the Nutrition Society, 2020, 79, .  | 0.4 | 0         |
| 185 | Multiblock methods in Analytical Chemistry. Brazilian Journal of Analytical Chemistry, 2021, 8, 16-21.   | 0.3 | O         |
| 186 | A longitudinal study of the effect of temperature modification in full-scale anaerobic digesters – dataset combining 16S rDNA gene sequencing, metagenomics, and metabolomics data. Data in Brief, 2022, 41, 107960. | 0.5 | 0         |