Romà Tauler

List of Publications by Year in descending order

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47 papers 1,958

279798 23 h-index 254184 43 g-index

48 all docs 48 docs citations

48 times ranked

2658 citing authors

#	Article	IF	CITATIONS
1	Comparison of the variable importance in projection (VIP) and of the selectivity ratio (SR) methods for variable selection and interpretation. Journal of Chemometrics, 2015, 29, 528-536.	1.3	402
2	Data analysis strategies for targeted and untargeted LC-MS metabolomic studies: Overview and workflow. TrAC - Trends in Analytical Chemistry, 2016, 82, 425-442.	11.4	240
3	Chemometrics in analytical chemistry—part II: modeling, validation, and applications. Analytical and Bioanalytical Chemistry, 2018, 410, 6691-6704.	3.7	102
4	Assessment of endocrine disruptors effects on zebrafish (Danio rerio) embryos by untargeted LC-HRMS metabolomic analysis. Science of the Total Environment, 2018, 635, 156-166.	8.0	97
5	Chemometrics in analytical chemistry—part I: history, experimental design and data analysis tools. Analytical and Bioanalytical Chemistry, 2017, 409, 5891-5899.	3.7	95
6	Detection of Olive Oil Adulteration Using FTâ€IR Spectroscopy and PLS with Variable Importance of Projection (VIP) Scores. JAOCS, Journal of the American Oil Chemists' Society, 2012, 89, 1807-1812.	1.9	90
7	Untargeted Comprehensive Two-Dimensional Liquid Chromatography Coupled with High-Resolution Mass Spectrometry Analysis of Rice Metabolome Using Multivariate Curve Resolution. Analytical Chemistry, 2017, 89, 7675-7683.	6.5	72
8	Is independent component analysis appropriate for multivariate resolution in analytical chemistry?. TrAC - Trends in Analytical Chemistry, 2012, 31, 134-143.	11.4	68
9	Application of Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) to remote sensing hyperspectral imaging. Analytica Chimica Acta, 2013, 762, 25-38.	5.4	58
10	Trilinearity and component interaction constraints in the multivariate curve resolution investigation of NO and O3 pollution in Barcelona. Analytical and Bioanalytical Chemistry, 2011, 399, 2015-2029.	3.7	50
11	Chemometric analysis of comprehensive two dimensional gas chromatography–mass spectrometry metabolomics data. Journal of Chromatography A, 2017, 1488, 113-125.	3.7	48
12	Influence of minerals on the taste of bottled and tap water: AÂchemometric approach. Water Research, 2013, 47, 693-704.	11.3	43
13	Metabolomic analysis of the effects of cadmium and copper treatment in Oryza sativa L. using untargeted liquid chromatography coupled to high resolution mass spectrometry and all-ion fragmentation. Metallomics, 2017, 9, 660-675.	2.4	43
14	LC-MS based metabolomics and chemometrics study of the toxic effects of copper on Saccharomyces cerevisiae. Metallomics, 2016, 8, 790-798.	2.4	42
15	Phenotypic malignant changes and untargeted lipidomic analysis of long-term exposed prostate cancer cells to endocrine disruptors. Environmental Research, 2015, 140, 18-31.	7.5	36
16	Chemometric analysis of comprehensive LC×LC-MS data: Resolution of triacylglycerol structural isomers in corn oil. Talanta, 2016, 160, 624-635.	5 . 5	34
17	Handling Different Spatial Resolutions in Image Fusion by Multivariate Curve Resolution-Alternating Least Squares for Incomplete Image Multisets. Analytical Chemistry, 2018, 90, 6757-6765.	6.5	31
18	Application of the area correlation constraint in the MCR-ALS quantitative analysis of complex mixture samples. Analytica Chimica Acta, 2020, 1113, 52-65.	5.4	31

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19	Multivariate Curve Resolution for Quantitative Analysis. Data Handling in Science and Technology, 2015, 29, 247-292.	3.1	30
20	Application of maximum likelihood multivariate curve resolution to noisy data sets. Journal of Chemometrics, 2013, 27, 34-41.	1.3	28
21	Exploring the interaction between O3 and NOx pollution patterns in the atmosphere of Barcelona, Spain using the MCR–ALS method. Science of the Total Environment, 2015, 517, 151-161.	8.0	26
22	Quantifying the Prediction Error in Analytical Multivariate Curve Resolution Studies of Multicomponent Systems. Analytical Chemistry, 2018, 90, 7040-7047.	6.5	26
23	Validation of the Regions of Interest Multivariate Curve Resolution (ROIMCR) procedure for untargeted LC-MS lipidomic analysis. Analytica Chimica Acta, 2018, 1025, 80-91.	5.4	25
24	Non-target protein analysis of samples from wastewater treatment plants using the regions of interest-multivariate curve resolution (ROIMCR) chemometrics method. Journal of Environmental Chemical Engineering, 2021, 9, 105752.	6.7	20
25	Untangling comprehensive two-dimensional liquid chromatography data sets using regions of interest and multivariate curve resolution approaches. TrAC - Trends in Analytical Chemistry, 2021, 137, 116207.	11.4	18
26	Compression of multidimensional NMR spectra allows a faster and more accurate analysis of complex samples. Chemical Communications, 2018, 54, 3090-3093.	4.1	17
27	Nâ∈BANDS: A new algorithm for estimating the extension of feasible bands in multivariate curve resolution of multicomponent systems in the presence of noise and rotational ambiguity. Journal of Chemometrics, 2021, 35, e3317.	1.3	17
28	Comparative analysis of 1H NMR and 1H–13C HSQC NMR metabolomics to understand the effects of medium composition in yeast growth. Analytical Chemistry, 2018, 90, 12422-12430.	6.5	16
29	Untargeted assignment and automatic integration of 1 H NMR metabolomic datasets using a multivariate curve resolution approach. Analytica Chimica Acta, 2017, 964, 55-66.	5.4	14
30	Deciphering the Underlying Metabolomic and Lipidomic Patterns Linked to Thermal Acclimation in <i>Saccharomyces cerevisiae</i> . Journal of Proteome Research, 2018, 17, 2034-2044.	3.7	14
31	Evaluation of the extension of rotation ambiguity associated to multivariate curve resolution solutions by the application of the MCR-BANDS method. Talanta, 2019, 202, 554-564.	5.5	14
32	Multivariate curve resolution of multiway data using the multilinearity constraint. Journal of Chemometrics, 2021, 35, e3279.	1.3	14
33	Assessment of the effects of As(III) treatment on cyanobacteria lipidomic profiles by LC-MS and MCR-ALS. Analytical and Bioanalytical Chemistry, 2016, 408, 5829-5841.	3.7	12
34	Local rank-based spatial information for improvement of remote sensing hyperspectral imaging resolution. Talanta, 2016, 146, 1-9.	5 . 5	12
35	Untargeted lipidomic analysis of primary human epidermal melanocytes acutely and chronically exposed to UV radiation. Molecular Omics, 2018, 14, 170-180.	2.8	11
36	Adverse Effects of Arsenic Uptake in Rice Metabolome and Lipidome Revealed by Untargeted Liquid Chromatography Coupled to Mass Spectrometry (LC-MS) and Regions of Interest Multivariate Curve Resolution. Separations, 2022, 9, 79.	2.4	10

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37	Non-targeted Gas Chromatography Orbitrap Mass Spectrometry qualitative and quantitative analysis of semi-volatile organic compounds in indoor dust using the Regions of Interest Multivariate Curve Resolution chemometrics procedure. Journal of Chromatography A, 2022, 1668, 462907.	3.7	9
38	Chemometric evaluation of different experimental conditions on wheat (Triticum aestivum L.) development using liquid chromatography mass spectrometry (LC–MS) profiles of benzoxazinone derivatives. Analytica Chimica Acta, 2012, 731, 24-31.	5.4	8
39	Chemometric evaluation of hydrophilic interaction liquid chromatography stationary phases: resolving complex mixtures of metabolites. Analytical Methods, 2017, 9, 774-785.	2.7	8
40	Extraction of climatic signals from fossil organic compounds in marine sediments up to 11.7Ma old (IODP-U1318). Analytica Chimica Acta, 2015, 879, 1-9.	5.4	7
41	Multivariate analysis of the operational parameters and environmental factors of an industrial solar pond. Solar Energy, 2021, 223, 113-124.	6.1	6
42	Understanding temporal and spatial changes of O3 or NO2 concentrations combining multivariate data analysis methods and air quality transport models. Science of the Total Environment, 2022, 806, 150923.	8.0	6
43	Monitoring biodiesel and its intermediates in transesterification reactions with multivariate curve resolution alternating least squares calibration models. Fuel, 2021, 283, 119275.	6.4	3
44	Quantification strategies for two-dimensional liquid chromatography datasets using regions of interest and multivariate curve resolution approaches. Talanta, 2022, 247, 123586.	5 . 5	3
45	An underground strategy to increase mercury tolerance in the salt marsh halophyte Juncus maritimus Lam.: Lipid remodelling and Hg restriction. Environmental and Experimental Botany, 2021, 191, 104619.	4.2	2
46	European Analytical Column No. 42. Analytical and Bioanalytical Chemistry, 2014, 406, 3525-3529.	3.7	0
47	European analytical column number 42. Accreditation and Quality Assurance, 2014, 19, 225-229.	0.8	O