Anna de Juan

List of Publications by Citations

148 papers	7,228 citations	41 h-index	82 g-index
158 ext. papers	7,924 ext. citations	5.2 avg, IF	6.28 L-index

#	Paper	IF	Citations
148	A graphical user-friendly interface for MCR-ALS: a new tool for multivariate curve resolution in MATLAB. *Chemometrics and Intelligent Laboratory Systems*, **2005**, 76, 101-110	3.8	852
147	Multivariate Curve Resolution (MCR) from 2000: Progress in Concepts and Applications. *Critical Reviews in Analytical Chemistry*, **2006**, 36, 163-176	5.2	501
146	MCR-ALS GUI 2.0: New features and applications. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 140, 1-12	3.8	466
145	Chemometrics applied to unravel multicomponent processes and mixtures: Revisiting latest trends in multivariate resolution. *Analytica Chimica Acta*, **2003**, 500, 195-210	6.6	448
144	Multivariate Curve Resolution (MCR). Solving the mixture analysis problem. *Analytical Methods*, **2014**, 6, 4964-4976	3.2	340
143	Combining hard- and soft-modelling to solve kinetic problems. *Chemometrics and Intelligent Laboratory Systems*, **2000**, 54, 123-141	3.8	259
142	Multivariate image analysis: A review with applications. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 107, 1-23	3.8	203
141	Comprehensive data analysis of femtosecond transient absorption spectra: A review. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, **2012**, 13, 1-27	16.4	200
140	Vibrational spectroscopic image analysis of biological material using multivariate curve resolution-alternating least squares (MCR-ALS). *Nature Protocols*, **2015**, 10, 217-40	18.8	190
139	Assessment of new constraints applied to the alternating least squares method. *Analytica Chimica Acta*, **1997**, 346, 307-318	6.6	175
138	Spectroscopic imaging and chemometrics: a powerful combination for global and local sample analysis. *TrAC - Trends in Analytical Chemistry*, **2004**, 23, 70-79	14.6	152
137	Comparison of three-way resolution methods for non-trilinear chemical data sets. *Journal of Chemometrics*, **2001**, 15, 749-771	1.6	152
136	Application of chemometric methods to environmental analysis of organic pollutants: A review. *Talanta*, **2010**, 80, 1052-67	6.2	102
135	Resolution and segmentation of hyperspectral biomedical images by multivariate curve resolution-alternating least squares. *Analytica Chimica Acta*, **2011**, 705, 182-92	6.6	91
134	Modeling temperature-dependent protein structural transitions by combined near-IR and mid-IR spectroscopies and multivariate curve resolution. *Analytical Chemistry*, **2003**, 75, 5592-601	7.8	85
133	Application of a combination of hard and soft modeling for equilibrium systems to the quantitative analysis of pH-modulated mixture samples. *Analytical Chemistry*, **2003**, 75, 641-7	7.8	84
132	Application of a novel resolution approach combining soft- and hard-modelling features to investigate temperature-dependent kinetic processes. *Analytica Chimica Acta*, **2001**, 442, 337-350	6.6	82

131	Factor analysis of hyphenated chromatographic data exploration, resolution and quantification of multicomponent systems. *Journal of Chromatography A*, **2007**, 1158, 184-95	4.5	80
130	Comparison between the direct trilinear decomposition and the multivariate curve resolution-alternating least squares methods for the resolution of three-way data sets. *Chemometrics and Intelligent Laboratory Systems*, **1998**, 40, 19-32	3.8	74
129	Use of local rank-based spatial information for resolution of spectroscopic images. *Journal of Chemometrics*, **2008**, 22, 291-298	1.6	74
128	Detection and resolution of intermediate species in protein folding processes using fluorescence and circular dichroism spectroscopies and multivariate curve resolution. *Analytical Chemistry*, **2002**, 74, 6031-9	7.8	70
127	Relevant aspects of quantification and sample heterogeneity in hyperspectral image resolution. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 117, 169-182	3.8	62
126	Photodegradation study of decabromodiphenyl ether by UV spectrophotometry and a hybrid hard- and soft-modelling approach. *Analytica Chimica Acta*, **2008**, 618, 18-28	6.6	62
125	Local rank analysis for exploratory spectroscopic image analysis. Fixed Size Image Window-Evolving Factor Analysis. *Chemometrics and Intelligent Laboratory Systems*, **2005**, 77, 64-74	3.8	59
124	Three-way data analysis applied to multispectroscopic monitoring of protein folding. *Analytica Chimica Acta*, **2001**, 446, 185-195	6.6	53
123	Purity assessment and resolution of tetracycline hydrochloride samples analysed using high-performance liquid chromatography with diode array detection. *Journal of Chromatography A*, **1999**, 832, 67-86	4.5	53
122	Multiset Data Analysis: Extended Multivariate Curve Resolution **2009**, 473-505		52
121	A mixed hard- and soft-modelling approach to study and monitor enzymatic systems in biological fluids. *Analytica Chimica Acta*, **2006**, 567, 245-254	6.6	52
120	Application of correlation constrained multivariate curve resolution alternating least-squares methods for determination of compounds of interest in biodiesel blends using NIR and UV-visible spectroscopic data. *Talanta*, **2014**, 125, 233-41	6.2	51
119	Chemometric tools for classification and elucidation of protein secondary structure from infrared and circular dichroism spectroscopic measurements. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 527-41	4.2	48
118	Hybrid hard- and soft-modeling applied to difference spectra. *Chemometrics and Intelligent Laboratory Systems*, **2007**, 89, 26-35	3.8	47
117	A mixed hard- and soft-modelling approach for the quantitative determination of oxipurines and uric acid in human urine. *Analytica Chimica Acta*, **2006**, 567, 236-244	6.6	47
116	Local rank exploratory analysis of evolving rank-deficient systems. *Chemometrics and Intelligent Laboratory Systems*, **2004**, 70, 11-21	3.8	47
115	Comprehensive liquid chromatography-ion-spray tandem mass spectrometry method for the identification and quantification of eight hydroxylated brominated diphenyl ethers in environmental matrices. *Journal of Mass Spectrometry*, **2007**, 42, 890-9	2.2	45
114	Monitoring polymorphic transformations by using in situ Raman hyperspectral imaging and image multiset analysis. *Analytica Chimica Acta*, **2014**, 819, 15-25	6.6	44

113	Use of Raman spectroscopy and chemometrics to distinguish blue ballpoint pen inks. *Forensic Science International*, **2015**, 249, 73-82	2.6	44
112	Quantification of paracetamol through tablet blister packages by Raman spectroscopy and multivariate curve resolution-alternating least squares. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 125, 58-66	3.8	43
111	Solvent classification based on solvatochromic parameters: a comparison with the Snyder approach. *TrAC - Trends in Analytical Chemistry*, **1997**, 16, 52-62	14.6	42
110	Application of the local regression method interval partial least-squares to the elucidation of protein secondary structure. *Analytical Biochemistry*, **2005**, 336, 231-42	3.1	42
109	Application of the needle algorithm for exploratory analysis and resolution of HPLC-DAD data. *Chemometrics and Intelligent Laboratory Systems*, **1996**, 33, 133-145	3.8	42
108	Determination of phenolic compounds and authentication of PDO Lambrusco wines by HPLC-DAD and chemometric techniques. *Analytica Chimica Acta*, **2013**, 761, 34-45	6.6	41
107	pH- and time-dependent hemoglobin transitions: a case study for process modelling. *Analytica Chimica Acta*, **2007**, 595, 198-208	6.6	41
106	Monitoring and modeling of protein processes using mass spectrometry, circular dichroism, and multivariate curve resolution methods. *Analytical Chemistry*, **2006**, 78, 4768-78	7.8	39
105	Characterization of methanol-water and acetonitrile-water association using multivariate curve resolution methods. *Analytical Chemistry*, **2000**, 72, 1956-63	7.8	37
104	Chromatographic and spectroscopic data fusion analysis for interpretation of photodegradation processes. *Journal of Chromatography A*, **2011**, 1218, 9260-8	4.5	36
103	Chemometric Tools for Image Analysis65-109		36
102	Solvatochromic parameters for binary mixtures and a correlation with equilibrium constants. Part I. Dioxane-water mixtures. *Journal of Solution Chemistry*, **1992**, 21, 147-162	1.8	35
101	Chemometric strategies to unmix information and increase the spatial description of hyperspectral images: a single-cell case study. *Analytical Chemistry*, **2013**, 85, 6303-11	7.8	33
100	Matrix augmentation for breaking rank-deficiency: A case study. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 80, 209-214	3.8	33
99	Comparison of PARAFAC2 and MCR-ALS for resolution of an analytical liquid dilution system. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 83, 13-25	3.8	33
98	Quantitation of Mixtures of Diprotic Organic Acids by FT-IR Flow Titrations and Multivariate Curve Resolution. *Applied Spectroscopy*, **2002**, 56, 40-50	3.1	32
97	Multivariate Curve Resolution: 50 years addressing the mixture analysis problem - A review. *Analytica Chimica Acta*, **2021**, 1145, 59-78	6.6	32
96	A soft-modeling approach to interpret thermodynamic and conformational transitions of polynucleotides. *Biophysical Journal*, **1997**, 73, 2937-48	2.9	31

95	Combining multiset resolution and segmentation for hyperspectral image analysis of biological tissues. *Analytica Chimica Acta*, **2015**, 881, 24-36	6.6	30
94	Multivariate curve resolution of rapid-scan FTIR difference spectra of quinone photoreduction in bacterial photosynthetic membranes. *Analytical and Bioanalytical Chemistry*, **2007**, 387, 1863-73	4.4	30
93	Two-Way Data Analysis: Multivariate Curve Resolution – Iterative Resolution Methods **2009**, 325-344		29
92	Distribution of a low dose compound within pharmaceutical tablet by using multivariate curve resolution on Raman hyperspectral images. *Journal of Pharmaceutical and Biomedical Analysis*, **2015**, 103, 35-43	3.5	28
91	Comparison of second-order multivariate methods for screening and determination of PAHs by total fluorescence spectroscopy. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 132, 63-74	3.8	28
90	Blending process modeling and control by multivariate curve resolution. *Talanta*, **2013**, 117, 492-504	6.2	27
89	Monitoring and interpretation of photoinduced biochemical processes by rapid-scan FTIR difference spectroscopy and hybrid hard and soft modeling. *Journal of Physical Chemistry B*, **2009**, 113, 6031-40	3.4	27
88	Multivariate Curve Resolution-Alternating Least Squares for Spectroscopic Data. *Data Handling in Science and Technology*, **2016**, 30, 5-51	2.7	27
87	Modeling strategies for pharmaceutical blend monitoring and end-point determination by near-infrared spectroscopy. *International Journal of Pharmaceutics*, **2014**, 473, 219-31	6.5	26
86	Multivariate Curve Resolution for Quantitative Analysis. *Data Handling in Science and Technology*, **2015**, 29, 247-292	2.7	26
85	Characterization of Reversed-Phase Liquid Chromatographic Stationary Phases Using Solvatochromism and Multivariate Curve Resolution. *Analytical Chemistry*, **1999**, 71, 5225-5234	7.8	26
84	Application of a sparseness constraint in multivariate curve resolution ´- Alternating least squares. *Analytica Chimica Acta*, **2018**, 1000, 100-108	6.6	25
83	Multivariate unmixing approaches on Raman images of plant cell walls: new insights or overinterpretation of results?. *Plant Methods*, **2018**, 14, 52	5.8	24
82	Introduction to Multivariate Curve Resolution **2009**, 249-259		24
81	Application of multivariate curve resolution to the temperature-induced unfolding of α-chymotrypsin. *Analytica Chimica Acta*, **2005**, 544, 159-166	6.6	24
80	Unravelling the Metabolic Progression of Breast Cancer Cells to Bone Metastasis by Coupling Raman Spectroscopy and a Novel Use of Mcr-Als Algorithm. *Analytical Chemistry*, **2018**, 90, 5594-5602	7.8	23
79	Relevant aspects of unmixing/resolution analysis for the interpretation of biological vibrational hyperspectral images. *TrAC - Trends in Analytical Chemistry*, **2017**, 94, 130-140	14.6	23
78	Three-way data analysis of pollutant degradation profiles monitored using liquid chromatography–diode array detection. *Journal of Chemometrics*, **1999**, 13, 331-341	1.6	23

77	Chemometrics description of measurement error structure: study of an ultrafast absorption spectroscopy experiment. *Analytica Chimica Acta*, **2009**, 642, 19-26	6.6	22
76	Factor analysis applied to the study of the effects of solvent composition and nature of the inert electrolyte on the protonation constants in dioxane-water mixtures. *Analytica Chimica Acta*, **1993**, 283, 548-558	6.6	22
75	Confocal Raman imaging and chemometrics applied to solve forensic document examination involving crossed lines and obliteration cases by a depth profiling study. *Analyst, The*, **2017**, 142, 1106-1118	5	21
74	Handling Different Spatial Resolutions in Image Fusion by Multivariate Curve Resolution-Alternating Least Squares for Incomplete Image Multisets. *Analytical Chemistry*, **2018**, 90, 6757-6765	7.8	21
73	Ubiquinol formation in isolated photosynthetic reaction centres monitored by time-resolved differential FTIR in combination with 2D correlation spectroscopy and multivariate curve resolution. *Analytical and Bioanalytical Chemistry*, **2011**, 399, 1999-2014	4.4	21
72	Chemometric strategies for the study of the complexation of Al(III) ions with model molecule of humic substances from UV-vis data sets. *Analytica Chimica Acta*, **2005**, 544, 337-344	6.6	21
71	Chemometric determination of PAHs in aerosol samples by fluorescence spectroscopy and second-order data analysis algorithms. *Journal of Chemometrics*, **2014**, 28, 260-271	1.6	20
70	Hybrid hard- and soft-modeling approach for the resolution of convoluted femtosecond spectrokinetic data. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 105, 74-82	3.8	20
69	A new matching image preprocessing for image data fusion. *Chemometrics and Intelligent Laboratory Systems*, **2017**, 164, 32-42	3.8	19
68	Screening and quantification of proteinaceous binders in medieval paints based on Fourier transform infrared spectroscopy and multivariate curve resolution alternating least squares. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 134, 148-157	3.8	19
67	Multivariate Curve Resolution Applied to Hyperspectral Imaging Analysis of Chocolate Samples. *Applied Spectroscopy*, **2015**, 69, 993-1003	3.1	19
66	Assessment of solvent parameters and their correlation with protonation constants in dioxane-water mixtures using factor analysis. *Chemometrics and Intelligent Laboratory Systems*, **1991**, 12, 29-38	3.8	19
65	Study of the photodegradation of 2-bromophenol under UV and sunlight by spectroscopic, chromatographic and chemometric techniques. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2012**, 910, 138-48	3.2	18
64	High-throughput carotenoid profiling using multivariate curve resolution. *Analytical and Bioanalytical Chemistry*, **2013**, 405, 5075-86	4.4	17
63	Focus on the potential of hybrid hard- and soft-MCR-ALS in time resolved spectroscopy. *Journal of Chemometrics*, **2008**, 22, 666-673	1.6	17
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60	Comprehensive description of the photodegradation of bromophenols using chromatographic monitoring and chemometric tools. *Talanta*, **2011**, 83, 1134-46	6.2	16

59	Experimental monitoring and data analysis tools for protein folding: study of steady-state evolution and modeling of kinetic transients by multitechnique and multiexperiment data fusion. *Analytica Chimica Acta*, **2009**, 632, 52-62	6.6	16
58	Multivariate curve resolution--alternating least squares applied to the investigation of ultrafast competitive photoreactions. *Analytica Chimica Acta*, **2013**, 788, 8-16	6.6	15
57	Multivariate soft-modeling to predict radiocesium soil-to-plant transfer. *Environmental Science & Technology*, **2008**, 42, 4029-36	10.3	14
56	Soft Modeling of Analytical Data **2000**,		14
55	Multivariate Curve Resolution **2006**, 417-474		13
54	Local rank-based spatial information for improvement of remote sensing hyperspectral imaging resolution. *Talanta*, **2016**, 146, 1-9	6.2	12
53	Multivariate Curve Resolution: A Different Way To Examine Chemical Data. *ACS Symposium Series*, **2015**, 95-128	0.4	11
52	New chemometric approach MCR-ALS to unmix EPR spectroscopic data from complex mixtures. *Journal of Magnetic Resonance*, **2014**, 248, 27-35	3	10
51	i-motif structures in long cytosine-rich sequences found upstream of the promoter region of the SMARCA4 gene. *Biochimie*, **2017**, 140, 20-33	4.6	9
50	Multivariate curve resolution for hyperspectral image analysis. *Data Handling in Science and Technology*, **2020**, 32, 115-150	2.7	9
49	Process modeling and control applied to real-time monitoring of distillation processes by near-infrared spectroscopy. *Analytica Chimica Acta*, **2017**, 985, 41-53	6.6	9
48	Study of time-dependent structural changes of laponite colloidal system by means of near-infrared spectroscopy and hybrid hard- and soft-modelling multivariate curve resolution alternating least squares. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 142, 285-292	3.8	9
47	Assessment of tissue-specific multifactor effects in environmental -omics studies of heterogeneous biological samples: Combining hyperspectral image information and chemometrics. *Talanta*, **2019**, 194, 390-398	6.2	9
46	Process Monitoring of Moisture Content and Mass Transfer Rate in a Fluidised Bed with a Low Cost Inline MEMS NIR Sensor. *Pharmaceutical Research*, **2020**, 37, 84	4.5	9
45	Study of conformational transitions of i-motif DNA using time-resolved fluorescence and multivariate analysis methods. *Nucleic Acids Research*, **2019**, 47, 6590-6605	20.1	8
44	Understanding the Formation of Heartwood in Larch Using Synchrotron Infrared Imaging Combined With Multivariate Analysis and Atomic Force Microscope Infrared Spectroscopy. *Frontiers in Plant Science*, **2019**, 10, 1701	6.2	8
43	Three-way curve resolution applied to the study of solvent effect on the thermodynamic and conformational transitions related to the protonation of polycytidylic acid. *Analytical Biochemistry*, **1997**, 249, 174-83	3.1	8
42	3D and 4D Image Fusion: Coping with Differences in Spectroscopic Modes among Hyperspectral Images. *Analytical Chemistry*, **2020**, 92, 9591-9602	7.8	7

41	Characterization of the polarity of reversed-phase liquid chromatographic stationary phases in the presence of 1-propanol using solvatochromism and multivariate curve resolution. *Analytical Chemistry*, **2001**, 73, 290-7	7.8	7
40	Determination of a mixture of gamma-emitting radionuclides using solid scintillation detectors and multivariate calibration. *Analytica Chimica Acta*, **1999**, 379, 121-133	6.6	7
39	Application of a self-modeling curve resolution approach to the study of solvent effects on the acid-base and copper (II)-complexing behavior of polyuridylic acid. *Journal of Inorganic Biochemistry*, **1996**, 63, 155-73	4.2	7
38	Correlation of acid-base properties of solutes with the polarity parameters and other solvatochromic parameters of dioxane-water mixtures. *Inorganica Chimica Acta*, **1991**, 187, 187-195	2.7	7
37	Data fusion strategies to combine sensor and multivariate model outputs for multivariate statistical process control. *Analytical and Bioanalytical Chemistry*, **2020**, 412, 2151-2163	4.4	7
36	MALDI imaging mass spectrometry and chemometric tools to discriminate highly similar colorectal cancer tissues. *Talanta*, **2020**, 208, 120455	6.2	7
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34	Extraction of pure spectral signatures and corresponding chemical maps from EPR imaging data sets: identifying defects on a CaF2 surface due to a laser beam exposure. *Analytical Chemistry*, **2015**, 87, 3929-35	7.8	6
33	Hyperspectral image analysis. When space meets Chemistry. *Journal of Chemometrics*, **2018**, 32, e2985	1.6	6
32	Two-Way Data Analysis: Evolving Factor Analysis **2009**, 261-274		6
31	Multi-way analysis for investigation of industrial pectin using an analytical liquid dilution system. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 84, 9-20	3.8	6
30	Data Fusion by Multivariate Curve Resolution. *Data Handling in Science and Technology*, **2019**, 205-233	2.7	5
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28	Multiset Data Analysis: Extended Multivariate Curve Resolution **2020**, 305-336		5
27	Effect of physicochemical factors and use of milk powder on milk rennet-coagulation: Process understanding by near infrared spectroscopy and chemometrics. *Food Control*, **2021**, 119, 107494	6.2	5
26	Preprocessing Tools Applied to Improve the Assessment of Aldrin Effects on Prostate Cancer Cells Using Raman Spectroscopy. *Applied Spectroscopy*, **2018**, 72, 489-500	3.1	5
25	Use of physiological information based on grayscale images to improve mass spectrometry imaging data analysis from biological tissues. *Analytica Chimica Acta*, **2019**, 1074, 69-79	6.6	4
24	ICRM-2011 international chemometrics research meeting. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 111, 66	3.8	4

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22	Systematic comparison and potential combination between multivariate curve resolution–alternating least squares (MCR-ALS) and band-target entropy minimization (BTEM). *Journal of Chemometrics*, **2018**, 32, e3000	1.6	3
21	Chemometric Tools for Image Analysis **2014**, 57-110		3
20	Multivariate Curve Resolution Methods for Food Chemistry. *Data Handling in Science and Technology*, **2013**, 28, 235-263	2.7	3
19	Linear Soft-Modeling: Introduction **2009**, 207-210		3
18	Introduction to Multivariate Curve Resolution **2020**, 85-94		3
17	Acid recovery from copper metallurgical process streams polluted with arsenic by diffusion dialysis. *Journal of Environmental Chemical Engineering*, **2021**, 9, 104692	6.8	3
16	Setting local rank constraints by orthogonal projections for image resolution analysis: application to the determination of a low dose pharmaceutical compound. *Analytica Chimica Acta*, **2015**, 892, 49-58	6.6	2
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14	Acid number, viscosity and end-point detection in a multiphase high temperature polymerisation process using an online miniaturised MEMS Fabry-Pérot interferometer. *Talanta*, **2021**, 224, 121735	6.2	2
13	Two-Way Data Analysis: Multivariate Curve Resolution, Iterative Methods **2019**, 153-171		2
12	SWiVIA - Sliding window variographic image analysis for real-time assessment of heterogeneity indices in blending processes monitored with hyperspectral imaging. *Analytica Chimica Acta*, **2021**, 1180, 338852	6.6	2
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6	Linear unmixing protocol for hyperspectral image fusion analysis applied to a case study of vegetal tissues. *Scientific Reports*, **2021**, 11, 18665	4.9	0

5   A Soft-Modelling Approach to Interpret PH-Dependent Thermodynamical and Conformational Transitions of Polynucleotides **1997**, 247-248

4   A New Strategy of Spectroscopic Monitoring and Interpretation of Biomacromolecular Processes **1997**, 621-622

3   Two-Way Data Analysis: Evolving Factor Analysis **2020**, 95-106

2   Introduction to Linear Soft-Modeling **2020**, 1-2

1   Autofluorescence of stingray skeletal cartilage: hyperspectral imaging as a tool for histological characterization. *Discover Materials*, **2021**, 1, 1