Alejandro C Olivieri

List of Publications by Year
in descending order

249 papers	9,420 citations	34076 52 h-index	56687 83 g-index
254 all docs	254 docs citations	254 times ranked	5151 citing authors

#	Article	IF	Citations
1	Quadrupolar effects transferred to spin-12 magic-angle spinning spectra of solids. Progress in Nuclear Magnetic Resonance Spectroscopy, 1992, 24, 435-456.	3.9	312
2	Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report). Pure and Applied Chemistry, 2006, 78, 633-661.	0.9	309
3	Second- and third-order multivariate calibration: data, algorithms and applications. TrAC - Trends in Analytical Chemistry, 2007, 26, 752-765.	5.8	294
4	Analytical Figures of Merit: From Univariate to Multiway Calibration. Chemical Reviews, 2014, 114, 5358-5378.	23.0	276
5	IUPAC-Consistent Approach to the Limit of Detection in Partial Least-Squares Calibration. Analytical Chemistry, 2014, 86, 7858-7866.	3.2	252
6	Practical guidelines for reporting results in single- and multi-component analytical calibration: A tutorial. Analytica Chimica Acta, 2015, 868, 10-22.	2.6	232
7	Analytical Advantages of Multivariate Data Processing. One, Two, Three, Infinity?. Analytical Chemistry, 2008, 80, 5713-5720.	3.2	206
8	MVC2: A MATLAB graphical interface toolbox for second-order multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 246-251.	1.8	197
9	MVC1: an integrated MatLab toolbox for first-order multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2004, 73, 189-197.	1.8	191
10	On a versatile second-order multivariate calibration method based on partial least-squares and residual bilinearization: Second-order advantage and precision properties. Journal of Chemometrics, 2005, 19, 253-265.	0.7	172
11	Second- and higher-order data generation and calibration: A tutorial. Analytica Chimica Acta, 2014, 806, 8-26.	2.6	152
12	Carbon-13 NMR and x-ray structure determination of 1-(arylazo)-2-naphthols. Intramolecular proton transfer between nitrogen and oxygen atoms in the solid state. Journal of the American Chemical Society, 1989, 111, 5525-5532.	6.6	129
13	Application of chemometric methods to environmental analysis of organic pollutants: A review. Talanta, 2010, 80, 1052-1067.	2.9	119
14	Enhanced Synchronous Spectrofluorometric Determination of Tetracycline in Blood Serum by Chemometric Analysis. Comparison of Partial Least-Squares and Hybrid Linear Analysis Calibrations. Analytical Chemistry, 1999, 71, 4361-4368.	3.2	105
15	Second-Order Advantage Achieved with Four-Way Fluorescence Excitation‒Emission‒Kinetic Data Processed by Parallel Factor Analysis and Trilinear Least-Squares. Determination of Methotrexate and Leucovorin in Human Urine. Analytical Chemistry, 2004, 76, 5657-5666.	3.2	105
16	A comparison of orthogonal signal correction and net analyte preprocessing methods. Theoretical and experimental study. Chemometrics and Intelligent Laboratory Systems, 2001, 56, 73-81.	1.8	103
17	A new and efficient variable selection algorithm based on ant colony optimization. Applications to near infrared spectroscopy/partial least-squares analysis. Analytica Chimica Acta, 2011, 699, 18-25.	2.6	100
18	Interference-Free Analysis Using Three-Way Fluorescence Data and the Parallel Factor Model. Determination of Fluoroquinolone Antibiotics in Human Serum. Analytical Chemistry, 2003, 75, 2640-2646.	3.2	97

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19	Simultaneous spectrophotometric-multivariate calibration determination of several components of ophthalmic solutions: phenylephrine, chloramphenicol, antipyrine, methylparaben and thimerosal. Talanta, 2000, 52, 909-920.	2.9	96
20	Computing Sensitivity and Selectivity in Parallel Factor Analysis and Related Multiway Techniques: The Need for Further Developments in Net Analyte Signal Theory. Analytical Chemistry, 2005, 77, 4936-4946.	3.2	96
21	Sensitivity Equation for Quantitative Analysis with Multivariate Curve Resolution-Alternating Least-Squares: Theoretical and Experimental Approach. Analytical Chemistry, 2012, 84, 8697-8706.	3.2	92
22	Trilinear least-squares and unfolded-PLS coupled to residual trilinearization: New chemometric tools for the analysis of four-way instrumental data. Chemometrics and Intelligent Laboratory Systems, 2006, 80, 77-86.	1.8	89
23	Substituent and solvent effects on the proton transfer equilibrium in anils and azo derivatives of naphthol. Multinuclear NMR study and theoretical calculations. Journal of Molecular Structure, 2004, 705, 1-9.	1.8	82
24	A review on second- and third-order multivariate calibration applied to chromatographic data. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012, 910, 22-30.	1.2	82
25	A review of multivariate calibration methods applied to biomedical analysis. Microchemical Journal, 2006, 82, 29-42.	2.3	81
26	Standard error of prediction in parallel factor analysis of three-way data. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 75-82.	1.8	71
27	A closed-form expression for computing the sensitivity in second-order bilinear calibration. Journal of Chemometrics, 2005, 19, 583-592.	0.7	71
28	Wavelength selection by net analyte signals calculated with multivariate factor-based hybrid linear analysis (HLA). A theoretical and experimental comparison with partial least-squares (PLS). Analyst, The, 1999, 124, 725-731.	1.7	70
29	Different strategies for the direct determination of amoxicillin in human urine by second-order multivariate analysis of kinetic–spectrophotometric data. Talanta, 2007, 71, 806-815.	2.9	70
30	Development of a novel strategy for preconcentration of antibiotic residues in milk and their quantitation by capillary electrophoresis. Talanta, 2010, 82, 213-221.	2.9	70
31	Second-Order Advantage Achieved by Unfolded-Partial Least-Squares/Residual Bilinearization Modeling of Excitation–Emission Fluorescence Data Presenting Inner Filter Effects. Analytical Chemistry, 2006, 78, 8051-8058.	3.2	69
32	Determination of five pesticides in juice, fruit and vegetable samples by means of liquid chromatography combined with multivariate curve resolution. Analytica Chimica Acta, 2014, 814, 23-30.	2.6	69
33	Simultaneous determination of rifampicin, isoniazid and pyrazinamide in tablet preparations by multivariate spectrophotometric calibration. Journal of Pharmaceutical and Biomedical Analysis, 1999, 20, 681-686.	1.4	67
34	Visible/near infrared-partial least-squares analysis of Brix in sugar cane juice. Chemometrics and Intelligent Laboratory Systems, 2010, 102, 100-109.	1.8	66
35	Development of novel formulations for Chagas' disease: Optimization of benznidazole chitosan microparticles based on artificial neural networks. International Journal of Pharmaceutics, 2009, 367, 140-147.	2.6	65
36	Study of quadrupole-perturbed quartets in the solid-state magic-angle spinning phosphorus-31 NMR spectra of phosphine-copper(I) complexes. 63Cu electric field gradients and anisotropy in the 31P,63Cu scalar coupling. Journal of the American Chemical Society, 1992, 114, 5758-5763.	6.6	64

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37	A Test Field for the Second-Order Advantage in Bilinear Least-Squares and Parallel Factor Analyses:Â Fluorescence Determination of Ciprofloxacin in Human Urine. Analytical Chemistry, 2004, 76, 2798-2806.	3.2	63
38	Spectrofluorometric determination of diclofenac in tablets and ointments. Journal of Pharmaceutical and Biomedical Analysis, 1999, 20, 587-590.	1.4	62
39	Simultaneous determination of levodopa and benserazide by stopped-flow injection analysis and three-way multivariate calibration of kinetic-spectrophotometric data. Journal of Pharmaceutical and Biomedical Analysis, 2004, 36, 541-547.	1.4	60
40	MVC3: A MATLAB graphical interface toolbox for third-order multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2012, 116, 9-16.	1.8	60
41	13C NMR spectroscopic and AM1 study of the intramolecular proton transfer in anils of salicylaldehyde and 2-hydroxynaphthalene-1-carbaldehyde. Journal of the Chemical Society Perkin Transactions II, 1994, , 1067-1070.	0.9	59
42	Wavelength Selection for Multivariate Calibration Using a Genetic Algorithm:â€‰ A Novel Initialization Strategy. Journal of Chemical Information and Computer Sciences, 2002, 42, 1146-1153.	2.8	59
43	Multiway Partial Least-Squares Coupled to Residual Trilinearization:â€‰ A Genuine Multidimensional Tool for the Study of Third-Order Data. Simultaneous Analysis of Procaine and Its Metabolite <i>p</i>-Aminobenzoic Acid in Equine Serum. Analytical Chemistry, 2007, 79, 6949-6958.	3.2	59
44	Phenolic profiling of grapes, fermenting samples and wines using UV-Visible spectroscopy with chemometrics. Food Control, 2018, 85, 11-22.	2.8	59
45	Multi-way chromatographic calibrationâ€"A review. Journal of Chromatography A, 2019, 1587, 2-13.	1.8	59
46	First- and second-order multivariate calibration applied to biological samples: determination of anti-inflammatories in serum and urine. Analytical and Bioanalytical Chemistry, 2002, 374, 451-459.	1.9	58
47	A new family of genetic algorithms for wavelength interval selection in multivariate analytical spectroscopy. Journal of Chemometrics, 2003, 17, 338-345.	0.7	57
48	Recent advances in analytical calibration with multi-way data. Analytical Methods, 2012, 4, 1876.	1.3	57
49	Application of the correlation constrained multivariate curve resolution alternating least-squares method for analyte quantitation in the presence of unexpected interferences using first-order instrumental data. Analyst, The, 2010, 135, 636.	1.7	56
50	New Developments for the Sensitivity Estimation in Four-Way Calibration with the Quadrilinear Parallel Factor Model. Analytical Chemistry, 2012, 84, 186-193.	3.2	56
51	High-resolution solid-state carbon-13 NMR spectra of porphine and 5,10,15-20-tetraalkylporphyrins: implications for the nitrogen-hydrogen tautomerization process. Journal of the American Chemical Society, 1988, 110, 336-342.	6.6	54
52	Tautomerism of representative aromatic Î±-hydroxy carbaldehyde anils as studied by spectroscopic methods and AM1 calculations. Synthesis of 10-hydroxyphenanthrene-9-carbaldehyde. Tetrahedron, 1995, 51, 4619-4626.	1.0	54
53	Evaluation of partial least-squares with second-order advantage for the multi-way spectroscopic analysis of complex biological samples in the presence of analyteâ€"background interactions. Analyst, The, 2006, 131, 718-723.	1.7	54
54	Feasibility of the determination of polycyclic aromatic hydrocarbons in edible oils via unfolded partial least-squares/residual bilinearization and parallel factor analysis of fluorescence excitation emission matrices. Talanta, 2013, 103, 361-370.	2.9	53

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55	Second-order advantage from kinetic-spectroscopic data matrices in the presence of extreme spectral overlapping. Analytica Chimica Acta, 2008, 614, 46-57.	2.6	52
56	New Robust Bilinear Least Squares Method for the Analysis of Spectral-pH Matrix Data. Applied Spectroscopy, 2005, 59, 926-933.	1.2	50
57	Standard addition analysis of fluoroquinolones in human serum in the presence of the interferent salicylate using lanthanide-sensitized excitation-time decay luminescence data and multivariate curve resolution. Talanta, 2009, 77, 1715-1723.	2.9	48
58	New Method for the Determination of Benzoic and Sorbic Acids in Commercial Orange Juices Based on Second-Order Spectrophotometric Data Generated by a pH Gradient Flow Injection Technique. Journal of Agricultural and Food Chemistry, 2004, 52, 2479-2484.	2.4	47
59	Four-way kinetic-excitation-emission fluorescence data processed by multi-way algorithms. Determination of carbaryl and 1-naphthol in water samples in the presence of fluorescent interferents. Analytica Chimica Acta, 2010, 677, 97-107.	2.6	47
60	Unfolded partial least-squares with residual quadrilinearization: A new multivariate algorithm for processing five-way data achieving the second-order advantage. Application to fourth-order excitation-emission-kinetic-pH fluorescence analytical data. Chemometrics and Intelligent Laboratory Systems, 2011, 109, 178-185.	1.8	47
61	Chemometrics coupled to vibrational spectroscopy and spectroscopic imaging for the analysis of solid-phase pharmaceutical products: A brief review on non-destructive analytical methods. TrAC - Trends in Analytical Chemistry, 2018, 108, 74-87.	5.8	47
62	Structural analysis of natural deep eutectic solvents. Theoretical and experimental study. Microchemical Journal, 2018, 143, 252-258.	2.3	47
63	Comparative chemometric analysis of fluorescence and near infrared spectroscopies for authenticity confirmation and geographical origin of Argentinean extra virgin olive oils. Food Control, 2019, 96, 22-28.	2.8	47
64	Chemometric processing of second-order liquid chromatographic data with UVâ€"vis and fluorescence detection. A comparison of multivariate curve resolution and parallel factor analysis 2. Analytica Chimica Acta, 2014, 842, 11-19.	2.6	46
65	Anthocyanins as markers for the classification of Argentinean wines according to botanical and geographical origin. Chemometric modeling of liquid chromatographyâ€"mass spectrometry data. Food Chemistry, 2015, 175, 174-180.	4.2	46
66	Determination of theophylline in blood serum by UV spectrophotometry and partial least-squares (PLS-1) calibration. Analytica Chimica Acta, 1999, 384, 95-103.	2.6	45
67	Four-Way Data Coupled to Parallel Factor Model Applied to Environmental Analysis: Â Determination of 2,3,7,8-Tetrachloro-dibenzo-para-dioxin in Highly Contaminated Waters by Solidâˆ'Liquid Extraction Laser-Excited Time-Resolved Shpol'skii Spectroscopy. Analytical Chemistry, 2005, 77, 2608-2616.	3.2	45
68	Simultaneous determination of phenobarbital and phenytoin in tablet preparations by multivariate spectrophotometric calibration. Talanta, 1998, 47, 103-108.	2.9	44
69	A variable-temperature solid-state carbon-13 CPMAS NMR analysis of meso-tetrapropylporphyrin and of octaethylporphyrin. Journal of the American Chemical Society, 1988, 110, 5651-5661.	6.6	42
70	Direct and simultaneous spectrofluorometric determination of naproxen and salicylate in human serum assisted by chemometric analysis. Analytica Chimica Acta, 2002, 471, 87-96.	2.6	42
71	Determination of pesticides and metabolites in wine by high performance liquid chromatography and second-order calibration methods. Journal of Chromatography A, 2007, 1148, 200-210.	1.8	42
72	Screening of Oil Samples on the Basis of Excitationâˆ'Emission Room-Temperature Phosphorescence Data and Multiway Chemometric Techniques. Introducing the Second-Order Advantage in a Classification Study. Analytical Chemistry, 2008, 80, 2789-2798.	3.2	42

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73	Two Multivariate Strategies Applied to Three-Way Kinetic Spectrophotometric Data for the Determination of Mixtures of the Pesticides Carbaryl and Chlorpyrifos. Applied Spectroscopy, 2004, 58, 83-90.	1.2	41
74	Nonlinear Four-Way Kinetic-Excitationâˆ'Emission Fluorescence Data Processed by a Variant of Parallel Factor Analysis and by a Neural Network Model Achieving the Second-Order Advantage: Malonaldehyde Determination in Olive Oil Samples. Analytical Chemistry, 2008, 80, 7248-7256.	3.2	41
75	Introduction to Multivariate Calibration. , 2018, , .		41
76	Solid-state electronic absorption, fluorescence and13C CPMAS NMR spectroscopic study of thermo- and photo-chromic aromatic Schiff bases. Journal of the Chemical Society Perkin Transactions II, 1996, , 2293-2296.	0.9	39
77	Complementary use of partial least-squares and artificial neural networks for the non-linear spectrophotometric analysis of pharmaceutical samples. Analytical and Bioanalytical Chemistry, 2002, 374, 460-465.	1.9	39
78	In vivo evaluation of albendazole microspheres for the treatment of Toxocara canis larva migrans. European Journal of Pharmaceutics and Biopharmaceutics, 2010, 75, 451-454.	2.0	39
79	Microcomputer simulation of solid-state13C NMR line shapes affected by quadrupolar nuclei. Magnetic Resonance in Chemistry, 1988, 26, 615-618.	1.1	38
80	Sustained prediction ability of net analyte preprocessing methods using reduced calibration sets. Theoretical and experimental study involving the spectrophotometric analysis of multicomponent mixtures. Analyst, The, 2001, 126, 1105-1112.	1.7	38
81	Chemometric assisted simultaneous spectrophotometric determination of four-component nasal solutions with a reduced number of calibration samples. Analytica Chimica Acta, 2002, 453, 289-300.	2.6	38
82	Design and optimization of a chemometrics-assisted spectrophotometric method for the simultaneous determination of levodopa and carbidopa in pharmaceutical products. Analytica Chimica Acta, 2005, 543, 192-198.	2.6	38
83	A road map for multi-way calibration models. Analyst, The, 2017, 142, 2862-2873.	1.7	38
84	Quadrupole effects of nuclei on the solid-state magic-angle spinning nuclear magnetic resonance spectra of nuclei Deviations from first-order theory and implications concerning the sign of the indirect coupling constant. Solid State Nuclear Magnetic Resonance, 1993, 2, 325-334.	1.5	37
85	Three-way partial least-squares/residual bilinearization study of second-order lanthanide-sensitized luminescence excitation-time decay data. Analytica Chimica Acta, 2008, 610, 186-195.	2.6	37
86	Analytical Figures of Merit for Partial Least-Squares Coupled to Residual Multilinearization. Analytical Chemistry, 2012, 84, 10823-10830.	3.2	37
87	Evaluation of complex spectral-pH three-way arrays by modified bilinear least-squares: determination of four different dyes in interfering systems. Analyst, The, 2005, 130, 1291.	1.7	35
88	Concerning the crystal structure of porphine: a proton pulsed and carbon-13 cross-polarization/magic-angle-spinning NMR study. Journal of the American Chemical Society, 1989, 111, 7001-7005.	6.6	33
89	Chemometrics assisted spectroscopic determination of vitamin B6, vitamin B12 and dexamethasone in injectables. Journal of Pharmaceutical and Biomedical Analysis, 2003, 31, 621-627.	1.4	33
90	Multiple response optimization of styreneâ€"butadiene rubber emulsion polymerization. Computers and Chemical Engineering, 2009, 33, 850-856.	2.0	33

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91	Development and validation of chemometrics-assisted spectrophotometry and micellar electrokinetic chromatography for the determination of four-component pharmaceuticals. Analytica Chimica Acta, 2003, 489, 77-84.	2.6	32
92	A versatile strategy for achieving the second-order advantage when applying different artificial neural networks to non-linear second-order data: Unfolded principal component analysis/residual bilinearization. Chemometrics and Intelligent Laboratory Systems, 2008, 92, 61-70.	1.8	32
93	A new modeling strategy for third-order fast high-performance liquid chromatographic data with fluorescence detection. Quantitation of fluoroquinolones in water samples. Analytical and Bioanalytical Chemistry, 2015, 407, 1999-2011.	1.9	32
94	The effect of data matrix augmentation and constraints in extended multivariate curve resolution–alternating least squares. Journal of Chemometrics, 2017, 31, e2875.	0.7	32
95	A simple approach to uncertainty propagation in preprocessed multivariate calibration. Journal of Chemometrics, 2002, 16, 207-217.	0.7	31
96	Analysis of amoxicillin in human urine by photo-activated generation of fluorescence excitation–emission matrices and artificial neural networks combined with residual bilinearization. Analytica Chimica Acta, 2007, 588, 192-199.	2.6	31
97	A novel second-order standard addition analytical method based on data processing with multidimensional partial least-squares and residual bilinearization. Analytica Chimica Acta, 2009, 651, 165-172.	2.6	31
98	Flow injection system for the on-line preconcentration of Pb by cloud point extraction coupled to USN–ICP OES. Microchemical Journal, 2010, 95, 306-310.	2.3	31
99	Analytical chemistry assisted by multi-way calibration: A contribution to green chemistry. Talanta, 2019, 204, 700-712.	2.9	31
100	The effects of interplay between quadrupolar, dipolar and shielding tensors on magic-angle spinning NMR spectra: shapes of spinning sidebands. Molecular Physics, 1996, 87, 669-677.	0.8	30
101	Chemometric resolution of fully overlapped CE peaks: Quantitation of carbamazepine in human serum in the presence of several interferences. Electrophoresis, 2008, 29, 4527-4537.	1.3	30
102	Spectroscopic and potentiometric study of aromatic α-hydroxy azo compounds and their copper(II) complexes. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 545-551.	1.7	29
103	A combined artificial neural network/residual bilinearization approach for obtaining the second-order advantage from three-way non-linear data. Journal of Chemometrics, 2005, 19, 615-624.	0.7	29
104	Rigorous Statistical Analysis of Errors in Chemical-Shift-Tensor Components Obtained from Spinning Sidebands in Solid-State NMR. Journal of Magnetic Resonance Series A, 1996, 123, 207-210.	1.6	28
105	Simultaneous multivariate spectrophotometric analysis of paracetamol and minor components (diphenhydramine or phenylpropanolamine) in tablet preparations. Journal of Pharmaceutical and Biomedical Analysis, 1999, 20, 255-261.	1.4	28
106	Solid–Liquid Extraction Room Temperature Phosphorimetry and Pattern Recognition for Screening Polycyclic Aromatic Hydrocarbons and Polychlorinated Biphenyls in Water Samples. Environmental Science & Technology, 2003, 37, 1385-1391.	4.6	28
107	An integrated approach to the simultaneous selection of variables, mathematical pre-processing and calibration samples in partial least-squares multivariate calibration. Talanta, 2013, 115, 755-760.	2.9	28
108	Novel augmented parallel factor model for four-way calibration of high-performance liquid chromatography–fluorescence excitation–emission data. Chemometrics and Intelligent Laboratory Systems, 2015, 141, 1-11.	1.8	28

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109	Fast spectrophotometric determination of fluoride in ground waters by flow injection using partial least-squares calibration. Analytica Chimica Acta, 2004, 512, 157-163.	2.6	27
110	When unfolding is better: unique success of unfolded partial least-squares regression with residual bilinearization for the processing of spectralâ€"pH data with strong spectral overlapping. Analysis of fluoroquinolones in human urine based on flow-injection pH-modulated synchronous fluorescence data matrices. Analyst, The, 2009, 134, 1682.	1.7	27
111	Second-Order Analyte Quantitation under Identical Profiles in One Data Dimension. A Dependency-Adapted Partial Least-Squares/Residual Bilinearization Method. Analytical Chemistry, 2010, 82, 4510-4519.	3.2	27
112	Sensitivity, Prediction Uncertainty, and Detection Limit for Artificial Neural Network Calibrations. Analytical Chemistry, 2016, 88, 7807-7812.	3.2	27
113	Generalized error-dependent prediction uncertainty in multivariate calibration. Analytica Chimica Acta, 2016, 903, 51-60.	2.6	27
114	Processing multi-way chromatographic data for analytical calibration, classification and discrimination: A successful marriage between separation science and chemometrics. TrAC - Trends in Analytical Chemistry, 2021, 134, 116128.	5.8	27
115	Simultaneous Multivariate Spectrophotometric Analysis of Binary and Ternary Mixtures of Sulfamethoxazole, Trimethoprim and Phenazopyridine in Tablets. Analytical Letters, 1999, 32, 1389-1401.	1.0	26
116	Spectrofluorimetric determination of phenylephrine in the presence of a large excess of paracetamol. Analytica Chimica Acta, 2000, 419, 159-168.	2.6	26
117	Quantifying the Prediction Error in Analytical Multivariate Curve Resolution Studies of Multicomponent Systems. Analytical Chemistry, 2018, 90, 7040-7047.	3.2	26
118	Ground- and excited-state prototropic tautomerism in anils of aromatic Î±-hydroxy aldehydes studied by electronic absorption, fluorescence and1H and13C NMR spectroscopies and semi-empirical calculations. Journal of Physical Organic Chemistry, 1995, 8, 713-720.	0.9	24
119	Multiresponse optimization of the properties of albendazoleâ€"chitosan microparticles. Journal of Pharmaceutical and Biomedical Analysis, 2008, 48, 802-807.	1.4	24
120	Spray drying formulation of albendazole microspheres by experimental design. *In vitroâ€"in vivo* studies. Drug Development and Industrial Pharmacy, 2015, 41, 244-252.	0.9	24
121	MVC3_GUI: A MATLAB graphical user interface for third-order multivariate calibration. An upgrade including new multi-way models. Chemometrics and Intelligent Laboratory Systems, 2018, 173, 21-29.	1.8	24
122	A simple theoretical treatment of quadrupolar effects on magic-angle-spinning solid-state NMR spectra of nuclei in the limit of large quadrupole coupling constants. Solid State Nuclear Magnetic Resonance, 1993, 1, 345-353.	1.5	23
123	Application of partial least-squares spectrophotometric-multivariate calibration to the determination of 2-sec-butyl-4,6-dinitrophenol (dinoseb) and 2,6-dinitro-p-cresol in industrial and water samples containing hydrocarbons. Analytica Chimica Acta, 2005, 553, 141-147.	2.6	22
124	Spectroscopic bilinear least-squares methods exploiting the second-order advantage. Theoretical and experimental study concerning accuracy, sensitivity and prediction error. Chemometrics and Intelligent Laboratory Systems, 2006, 80, 99-108.	1.8	22
125	A multiway approach for classification and characterization of rabbit liver apothioneins by CEâ€"ESIâ€"MS. Electrophoresis, 2008, 29, 4355-4367.	1.3	22
126	Multivariate curve-resolution analysis of pesticides in water samples from liquid chromatographicâ€"diode array data. Talanta, 2011, 83, 1173-1180.	2.9	22

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127	Classification of olive oils according to their cultivars based on second-order data using LC-DAD. Talanta, 2019, 195, 69-76.	2.9	22
128	Simultaneous Determination of Timolol Maleate and Pilocarpine Hydrochloride in Ophthalmic Solutions by First Derivative UV Spectrophotometry and PLS-1 Multivariate Calibration. Analytical Letters, 1999, 32, 2019-2033.	1.0	21
129	Experimental study of non-linear second-order analytical data with focus on the second-order advantage. Analyst, The, 2007, 132, 654-663.	1.7	21
130	Simultaneous multiresponse optimization applied to epinastine determination in human serum by using capillary electrophoresis. Analytica Chimica Acta, 2007, 595, 310-318.	2.6	20
131	Time dependence of the aroma pattern emitted by an encapsulated essence studied by means of electronic noses and chemometric analysis. Food Research International, 2010, 43, 797-804.	2.9	20
132	Determination of tributyltin at parts-per-trillion levels in natural waters by second-order multivariate calibration and fluorescence spectroscopy. Microchemical Journal, 2013, 106, 95-101.	2.3	20
133	SRO_ANN: An integrated MatLab toolbox for multiple surface response optimization using radial basis functions. Chemometrics and Intelligent Laboratory Systems, 2017, 171, 198-206.	1.8	20
134	Determination of three aspirin metabolites in human urine by derivative synchronous spectrofluorimetry. Analyst, The, 1995, 120, 443-445.	1.7	19
135	A new and consistent parameter for measuring the quality of multivariate analytical methods: Generalized analytical sensitivity. Analytica Chimica Acta, 2016, 933, 43-49.	2.6	19
136	A down-to-earth analyst view of rotational ambiguity in second-order calibration with multivariate curve resolutionÂâˆ’ a tutorial. Analytica Chimica Acta, 2021, 1156, 338206.	2.6	19
137	13C CPMAS NMR study of solid arylazonaphthols. Evidence of 13C,14N self-decoupling induced by a solid-state proton transfer reaction. Journal of the Chemical Society Perkin Transactions II, 1993, , 1783-1786.	0.9	18
138	Residual Dipolar (35,37 Cl, 13 C) Coupling in Solid Sodium Chloroacetates. A Combined Variable-Temperature 35 Cl NQR and Variable-Field 13 C MAS NMR Study. Journal of Magnetic Resonance Series A, 1995, 116, 244-250.	1.6	18
139	Simultaneous spectrofluorometric determination of oxatomide and phenylephrine in the presence of a large excess of paracetamol. Analytica Chimica Acta, 2001, 439, 87-94.	2.6	18
140	A 13C solid-state NMR study of the structure and the dynamics of the polymorphs of sulphanilamide. Molecular Physics, 1990, 70, 563-579.	0.8	17
141	Artificial neural networks study of the catalytic reduction of resazurin: stopped-flow injection kinetic-spectrophotometric determination of Cu(II) and Ni(II). Analytica Chimica Acta, 2005, 528, 275-284.	2.6	17
142	Residual bilinearization combined with kernel-unfolded partial least-squares: A new technique for processing non-linear second-order data achieving the second-order advantage. Chemometrics and Intelligent Laboratory Systems, 2010, 100, 127-135.	1.8	17
143	Interpretation of matrix chromatographic-spectral data modeling with parallel factor analysis 2 and multivariate curve resolution. Journal of Chromatography A, 2019, 1604, 460502.	1.8	17
144	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.	0.7	17

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145	C,O atomic motion associated with solid-state proton transfer in enolic 1,3-diketones. Journal of Molecular Structure, 1992, 274, 215-222.	1.8	16
146	Ground and excited state proton transfer in intramolecularly hydrogen bonded aromatic α-hydroxy azo, aldehydes and their derivatives. Journal of Molecular Structure, 1997, 415, 115-121.	1.8	16
147	Determination of the Active Principle in a Syrup by Spectrophotometry and Principal Component Regression Analysis. An Advanced Undergraduate Experiment Involving Chemometrics. Journal of Chemical Education, 2000, 77, 1330.	1.1	16
148	Sample-specific standard prediction errors in three-way parallel factor analysis (PARAFAC) exploiting the second-order advantage. Journal of Chemometrics, 2004, 18, 363-371.	0.7	16
149	A systematic study on the effect of noise and shift on multivariate figures of merit of second-order calibration algorithms. Analytica Chimica Acta, 2017, 952, 18-31.	2.6	16
150	Why should the pharmaceutical industry claim for the implementation of second-order chemometric models—A critical review. Journal of Pharmaceutical and Biomedical Analysis, 2020, 179, 112965.	1.4	16
151	SIMULTANEOUS MULTIVARIATE SPECTROPHOTOMETRIC ANALYSIS OF EAR DROPS CONTAINING A TERNARY MIXTURE OF ANTIPYRINE, SULFATHIAZOLE, AND RIVANOL. Analytical Letters, 2001, 34, 2077-2088.	1.0	15
152	Design, Characterization, and In Vitro Evaluation of Antifungal Polymeric Films. AAPS PharmSciTech, 2013, 14, 64-73.	1.5	15
153	Strategy To Obtain Accurate Analytical Solutions in Second-Order Multivariate Calibration with Curve Resolution Methods. Analytical Chemistry, 2018, 90, 9725-9733.	3.2	15
154	MVC1_GUI: A MATLAB graphical user interface for first-order multivariate calibration. An upgrade including artificial neural networks modelling. Chemometrics and Intelligent Laboratory Systems, 2020, 206, 104162.	1.8	15
155	Sensitivity for Multivariate Calibration Based on Multilayer Perceptron Artificial Neural Networks. Analytical Chemistry, 2020, 92, 12265-12272.	3.2	15
156	Stereoselective synthesis of the novel bisnorditerpene grindelistrictic acid, isolated from Grindelia stricta. Journal of Organic Chemistry, 1986, 51, 2824-2826.	1.7	14
157	Solid State NMR of Drugs: Soluble Aspirin. Analytical Letters, 1987, 20, 1657-1666.	1.0	14
158	Urea-phosphoric acid complex studied by variable temperature 31P NMR spectroscopy and semiempirical calculations. Journal of Physics and Chemistry of Solids, 1996, 57, 1183-1190.	1.9	14
159	Net Analyte Preprocessing: A New and Versatile Multivariate Calibration Technique. Analysis of Mixtures of Rubber Antioxidants by NIR Spectroscopy. Journal of Near Infrared Spectroscopy, 2001, 9, 245-254.	0.8	14
160	A New Genetic Algorithm Applied to the near Infrared Analysis of Gasolines. Journal of Near Infrared Spectroscopy, 2004, 12, 85-91.	0.8	14
161	Structural and ^{14}N EFG Information on Solid Imidazole by ^{13}C CP/MAS NMR Data. Spectroscopy Letters, 1991, 24, 895-907.	0.5	13
162	Second-order quadrupolar effects for directly bonded and remote ^{13}C–$^{79/81}Br$ spin pairs in high-resolution ^{13}C NMR spectra of solids. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3167-3176.	1.7	13

#	Article	IF	Citations
163	Random Error Analysis in the Determination of Equilibrium Constants of Very Stable Metal Complexes.. Analytical Letters, 1997, 30, 1967-1980.	1.0	13
164	Estimation of the composition of recombinant human erythropoietin mixtures using capillary electrophoresis and multivariate calibration methods. Electrophoresis, 2006, 27, 4008-4015.	1.3	13
165	Chemometric modeling of kinetic-fluorescent third-order data for thiamine determination in multivitamin complexes. Microchemical Journal, 2016, 128, 42-46.	2.3	13
166	Online Third-Order Liquid Chromatographic Data with Native and Photoinduced Fluorescence Detection for the Quantitation of Organic Pollutants in Environmental Water. ACS Omega, 2018, 3, 15771-15779.	1.6	13
167	Second‐order multivariate calibration with the extended bilinear model: Effect of initialization, constraints, and composition of the calibration set on the extent of rotational ambiguity. Journal of Chemometrics, 2020, 34, e3130.	0.7	13
168	Initialization effects in two-component second-order multivariate calibration with the extended bilinear model. Analytica Chimica Acta, 2020, 1125, 169-176.	2.6	13
169	Stereospecific transformation of grindelic acid into the antifeedant 6.alpha.-hydroxygrindelic acid, its 6.beta.-epimer, and other related natural diterpene acids. Journal of Organic Chemistry, 1984, 49, 4984-4988.	1.7	12
170	Total Fluorescence and Zero-Crossing First-Derivative Synchronous Fluorescence Determination Of Acetylsalicylic Acid Metabolites in Biological Fluids. Analytical Letters, 1993, 26, 247-257.	1.0	12
171	Determination of the minor component bromhexine in cotrimoxazole-containing tablets by absorption spectrophotometry and partial least-squares (PLS-1) multivariate calibration. Journal of Pharmaceutical and Biomedical Analysis, 2000, 23, 591-595.	1.4	12
172	Near-infrared spectroscopic determination of antioxidants and organic acids in rubbers assisted by a new multivariate calibration method based on direct orthogonalization. Analyst, The, 2002, 127, 304-309.	1.7	12
173	Improvement of residual bilinearization by particle swarm optimization for achieving the second‐order advantage with unfolded partial least‐squares. Journal of Chemometrics, 2007, 21, 557-566.	0.7	12
174	Recent advances in analytical figures of merit: heteroscedasticity strikes back. Analytical Methods, 2017, 9, 739-743.	1.3	12
175	EPSILON: a versatile microcomputer program for the spectrophotometric data analysis of metal‐ligand equilibria. Computers & Chemistry, 1998, 22, 161-168.	1.2	11
176	Principal component analysis-adaptive neuro-fuzzy inference systems (ANFISs) for the simultaneous spectrophotometric determination of three metals in water samples. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 608-614.	2.0	11
177	Determination of enantiomeric composition of ibuprofen in pharmaceutical formulations by partial least-squares regression of strongly overlapped chromatographic profiles. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012, 910, 78-83.	1.2	11
178	Multi-way figures of merit in the presence of heteroscedastic and correlated instrumental noise: Unfolded partial least-squares with residual multi-linearization. Chemometrics and Intelligent Laboratory Systems, 2016, 158, 200-209.	1.8	11
179	A New Parameter for Measuring the Prediction Uncertainty Produced by Rotational Ambiguity in Second-Order Calibration with Multivariate Curve Resolution. Analytical Chemistry, 2020, 92, 9118-9123.	3.2	11
180	Magic-angle-spinning 31P NMR spectra of solid dihydrogen phosphates. Solid State Nuclear Magnetic Resonance, 1992, 1, 205-210.	1.5	10

#	Article	IF	Citations
181	Deuterium isotope effects on31P NMR parameters: hydrogen bonding in a solid urea–phosphoric acid adduct. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 5047-5050.	1.7	10
182	Solid state NMR sideband shape simulations for any spinning angle and speed. First order calculation of residual dipolar coupling to quadrupolar nuclei. Solid State Nuclear Magnetic Resonance, 1997, 10, 19-24.	1.5	10
183	Optimization of the hydrolysis of lignocellulosic residues by using radial basis functions modeling and particle swarm optimization. Biochemical Engineering Journal, 2013, 80, 1-9.	1.8	10
184	Second-order advantage obtained from standard addition first-order instrumental data and multivariate curve resolution-alternating least squares. Calculation of the feasible bands of results. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 721-730.	2.0	10
185	Error Covariance Penalized Regression: A novel multivariate model combining penalized regression with multivariate error structure. Analytica Chimica Acta, 2018, 1011, 20-27.	2.6	10
186	On second-order calibration based on multivariate curve resolution in the presence of highly overlapped profiles. Analytica Chimica Acta, 2020, 1096, 53-60.	2.6	10
187	SIMULTANEOUS DETERMINATION OF NICOTINAMIDE AND INOSINE IN OPHTHALMIC SOLUTIONS BY UV SPECTROPHOTOMETRY AND PLS-1 MULTIVARIATE CALIBRATION. Analytical Letters, 2001, 34, 363-376.	1.0	9
188	Uncovering interactions in Plackett–Burman screening designs applied to analytical systems. A Monte Carlo ant colony optimization approach. Talanta, 2012, 97, 242-248.	2.9	9
189	The effect of constraints on the analytical figures of merit achieved by extended multivariate curve resolution-alternating least-squares. Analytica Chimica Acta, 2018, 1003, 10-15.	2.6	9
190	Multivariate Calibration: A Powerful Tool in Pharmaceutical Analysis. Current Pharmaceutical Analysis, 2005, 1, 145-154.	0.3	9
191	Developing and Implementing an R Shiny Application to Introduce Multivariate Calibration to Advanced Undergraduate Students. Journal of Chemical Education, 2020, 97, 1176-1180.	1.1	8
192	Solution of acid-base equilibria by successive approximations. Journal of Chemical Education, 1990, 67, 229.	1.1	7
193	Rapid Determination of Paracetamol in Blood Serum Samples by First-Derivative UV Absorption Spectroscopy. Analytical Letters, 1995, 28, 2219-2226.	1.0	7
194	Teaching Chemometrics with a Bioprocess: Analytical Methods Comparison Using Bivariate Linear Regression. The Chemical Educator, 2002, 7, 265-269.	0.0	7
195	Recent Applications of First- and Second-Order Multivariate Calibration to Analytical Chemistry. Journal of AOAC INTERNATIONAL, 2014, 97, 39-49.	0.7	7
196	Unfolded and Multiway Partial Least-Squares with Residual Multilinearization. Data Handling in Science and Technology, 2015, 29, 365-397.	3.1	7
197	Figures of Merit in Multiway Calibration. Data Handling in Science and Technology, 2015, 29, 541-575.	3.1	7
198	A novel application of nylon membranes for tributyltin determination in complex environmental samples by fluorescence spectroscopy and multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2015, 148, 77-84.	1.8	7

#	Article	IF	Citations
199	Interference-free calibration with first-order instrumental data and multivariate curve resolution. When and why?. Analytica Chimica Acta, 2021, 1161, 338465.	2.6	7
200	Achieving the analytical second-order advantage with non-bilinear second-order data. Analytica Chimica Acta, 2021, 1181, 338911.	2.6	7
201	Chromatographic Applications in the Multi-Way Calibration Field. Molecules, 2021, 26, 6357.	1.7	7
202	Evaluation of the ambiguity in second-order analytical calibration based on multivariate curve resolution. A tutorial. Microchemical Journal, 2022, 179, 107455.	2.3	7
203	An extension of the Beierbeck and Saunders parameters for the semiempirical calculation of the 13C nuclear magnetic resonance chemical shifts: the gauche-$\hat{I}3$(X) effect in epoxides. Canadian Journal of Chemistry, 1986, 64, 552-555.	0.6	6
204	Semiempirical calculation of 13C nuclear magnetic resonance chemical shifts of acyclic hydrocarbons. Application to the stereochemical analysis of steroidal side chains. Canadian Journal of Chemistry, 1988, 66, 71-75.	0.6	6
205	Conformational analysis of the 4a-methyl octahydrophenanthrene system. A spectroscopic and theoretical approach.. Tetrahedron, 1989, 45, 4951-4960.	1.0	6
206	13C CP/MAS NMR of a 13Cî—¸2H residual dipolar coupled pair. Solid State Nuclear Magnetic Resonance, 1996, 7, 121-125.	1.5	6
207	Chemometric modeling of organic contaminant sources in surface waters of a mediterranean river basin. Environmental Sciences: Processes and Impacts, 2014, 16, 124-134.	1.7	6
208	Unfolded and Multiway Partial Least-Squares with Residual Multilinearization. Data Handling in Science and Technology, 2015, 29, 347-363.	3.1	6
209	Multivariate curve resolution applied to kinetic-spectroscopic data matrices: Dye determination in foods by means of enzymatic oxidation. Talanta, 2017, 169, 189-194.	2.9	6
210	Maximum likelihood unfolded principal component regression with residual bilinearization (MLU-PCR/RBL) for second-order multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2017, 170, 51-57.	1.8	6
211	Complex numbers-partial least-squares applied to the treatment of electrochemical impedance spectroscopy data. Analytica Chimica Acta, 2019, 1080, 1-11.	2.6	6
212	Using chemometric tools to investigate the quality of three- and four-way liquid chromatographic data obtained with two different fluorescence detectors and applied to the determination of quinolone antibiotics in animal tissues. Chemometrics and Intelligent Laboratory Systems, 2020, 199, 103972.	1.8	6
213	Estimating the boundaries of the feasible profiles in the bilinear decomposition of multi-component data matrices. Chemometrics and Intelligent Laboratory Systems, 2021, 216, 104387.	1.8	6
214	Calculation of solubilities of carbonates and phosphates in water as influenced by competitive acid-base reactions. Journal of Chemical Education, 1990, 67, 934.	1.1	5
215	Proton transfer and Cu(II) binuclear complexes of 1,4-bis-p-sulfonylazo-2,3-dihydroxynaphthalene: a spectroscopic and potentiometric study in aqueous solution. Journal of Molecular Structure, 1997, 435, 199-206.	1.8	5
216	Errors in chemical shift tensor components and orientation in the molecular frame as obtained from MAS NMR spinning sideband analysis. Solid State Nuclear Magnetic Resonance, 1998, 11, 181-187.	1.5	5

#	Article	IF	Citations
217	Analytical Figures of Merit. , 2014, , 93-107.		5
218	Calibration Scenarios. , 2014, , 1-9.		5
219	Sensitivity and generalized analytical sensitivity expressions for quantitative analysis using convolutional neural networks. Analytica Chimica Acta, 2022, 1192, 338697.	2.6	5
220	How noise affects the band boundaries in multivariate curve resolution. Chemometrics and Intelligent Laboratory Systems, 2022, 220, 104472.	1.8	5
221	Model Studies for the Synthesis of Erigerol Synthesis of 1-Deoxy-13-Epierigerol from Grindelic Acid. Synthetic Communications, 1987, 17, 1727-1733.	1.1	4
222	Zero-crossing first and second derivative synchronous fluorescence spectroscopic determination of aspirin metabolites in urine. Journal of Pharmaceutical and Biomedical Analysis, 1994, 12, 1333-1335.	1.4	4
223	Retrieving31P Chemical-Shift-Tensor Information for Dihydrogen Phosphates in the Presence of Homonuclear31Pâ€œ31P Dipolar Coupling. Journal of Magnetic Resonance, 1997, 126, 138-141.	1.2	4
224	Partial Least-Squares with Residual Bilinearization. , 2014, , 157-195.		4
225	Contribution to second-order calibration based on multivariate curve resolution with and without previous chromatographic synchronization. Analytica Chimica Acta, 2019, 1078, 8-15.	2.6	4
226	A simple computer program for the calculation of 13C-NMR chemical shifts. Journal of Chemical Education, 1989, 66, 53.	1.1	3
227	Microcomputer program based on the Beierbeck-Saunders approach for the prediction of 13C-NMR chemical shifts in acyclic hydrocarbons. Analytica Chimica Acta, 1990, 233, 315-319.	2.6	3
228	14N Quadrupole Interactions in Nitrogen-Containing Ceramics. Effects on 29Si NMR Line Shapes and Structural Implications. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1992, 47, 39-44.	0.7	3
229	Retrieval of solid-state 31P nuclear magnetic resonance (NMR) chemical shielding parameters: proposal of an approach concerning variable-temperature 31P NMR mass spectra of urea phosphate and comparison of different methods. Solid State Nuclear Magnetic Resonance, 1994, 3, 163-170.	1.5	3
230	Simultaneous Determination of Two Antibiotics in Tablets by Spectrophotometry and Principal Component Regression (PCR) Analysis. An Advanced Undergraduate Experiment Involving Chemometrics. The Chemical Educator, 2000, 5, 236-241.	0.0	3
231	Experimental Three-way/Second-order Data. , 2014, , 27-45.		3
232	The Optimum Number of Latent Variables. , 2018, , 87-101.		3
233	Shifting of the keto-enol equilibrium in 1,3-diphenyl-1,3-propanedione by methyl substitution. An AM1 study. Computational and Theoretical Chemistry, 1994, 309, 59-64.	1.5	2
234	Illustrating rotating-frame (T1?) NMR relaxation with a microcomputer. Concepts in Magnetic Resonance, 1998, 10, 157-166.	1.3	2

#	Article	IF	Citations
235	Determination of Equilibrium Constants of Metal Complexes from Spectrophotometric Measurements. An Undergraduate Laboratory Experiment. Journal of Chemical Education, 1999, 76, 1277.	1.1	2
236	Parallel Factor Analysis. , 2014, , 109-125.		2
237	Chemometrics and Multivariate Calibration. , 2018, , 1-17.		2
238	Analytical Figures of Merit. , 2018, , 159-177.		2
239	FiguresÂof Merit. , 2020, , 441-463.		2
240	Three-way/Second-order StandardÂAddition. , 2014, , 197-216.		1
241	Mathematical Pre-processing. , 2018, , 139-158.		1
242	On the signal contribution function with respect to different norms. Journal of Chemometrics, 2021, 35, e3363.	0.7	1
243	Another method for solving equations in acid-base calculations. Journal of Chemical Education, 1983, 60, 911.	1.1	0
244	Comment on the equilibrium assumption in chemical kinetics. Journal of Chemical Education, 1987, 64, 1002.	1.1	0
245	Third-order/Four-way CalibrationÂand Beyond. , 2014, , 217-232.		0
246	MVC1: Software for Multivariate Calibration. , 2018, , 179-205.		0
247	The Classical Least-Squares Model. , 2018, , 19-38.		0
248	The Partial Least-Squares Model. , 2018, , 103-121.		0
249	Statistics and Food Quality. , 2021, , 362-386.		0