

# Alejandro C Olivieri

## List of Publications by Citations

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247  
papers

8,030  
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49  
h-index

77  
g-index

254  
ext. papers

8,566  
ext. citations

5.2  
avg, IF

6.7  
L-index

#	Paper	IF	Citations
247	Quadrupolar effects transferred to spin-12 magic-angle spinning spectra of solids. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , <b>1992</b> , 24, 435-456	10.4	282
246	Second- and third-order multivariate calibration: data, algorithms and applications. <i>TrAC - Trends in Analytical Chemistry</i> , <b>2007</b> , 26, 752-765	14.6	272
245	Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report). <i>Pure and Applied Chemistry</i> , <b>2006</b> , 78, 633-661	2.1	265
244	Analytical figures of merit: from univariate to multiway calibration. <i>Chemical Reviews</i> , <b>2014</b> , 114, 5358-788.1	88.1	215
243	MVC2: A MATLAB graphical interface toolbox for second-order multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2009</b> , 96, 246-251	3.8	181
242	Analytical advantages of multivariate data processing. One, two, three, infinity?. <i>Analytical Chemistry</i> , <b>2008</b> , 80, 5713-20	7.8	181
241	IUPAC-consistent approach to the limit of detection in partial least-squares calibration. <i>Analytical Chemistry</i> , <b>2014</b> , 86, 7858-66	7.8	177
240	MVC1: an integrated MatLab toolbox for first-order multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2004</b> , 73, 189-197	3.8	168
239	Practical guidelines for reporting results in single- and multi-component analytical calibration: a tutorial. <i>Analytica Chimica Acta</i> , <b>2015</b> , 868, 10-22	6.6	165
238	On a versatile second-order multivariate calibration method based on partial least-squares and residual bilinearization: Second-order advantage and precision properties. <i>Journal of Chemometrics</i> , <b>2005</b> , 19, 253-265	1.6	157
237	Second- and higher-order data generation and calibration: a tutorial. <i>Analytica Chimica Acta</i> , <b>2014</b> , 806, 8-26	6.6	139
236	Carbon-13 NMR and x-ray structure determination of 1-(arylozo)-2-naphthols. Intramolecular proton transfer between nitrogen and oxygen atoms in the solid state. <i>Journal of the American Chemical Society</i> , <b>1989</b> , 111, 5525-5532	16.4	110
235	Application of chemometric methods to environmental analysis of organic pollutants: A review. <i>Talanta</i> , <b>2010</b> , 80, 1052-67	6.2	102
234	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. <i>Analytical Chemistry</i> , <b>2004</b> , 76, 5657-66	7.8	99
233	A comparison of orthogonal signal correction and net analyte preprocessing methods. Theoretical and experimental study. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2001</b> , 56, 73-81	3.8	92
232	Enhanced synchronous spectrofluorometric determination of tetracycline in blood serum by chemometric analysis. Comparison of partial least-squares and hybrid linear analysis calibrations. <i>Analytical Chemistry</i> , <b>1999</b> , 71, 4361-8	7.8	91
231	Computing sensitivity and selectivity in parallel factor analysis and related multiway techniques: the need for further developments in net analyte signal theory. <i>Analytical Chemistry</i> , <b>2005</b> , 77, 4936-46	7.8	90

230	Sensitivity equation for quantitative analysis with multivariate curve resolution-alternating least-squares: theoretical and experimental approach. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 8697-706	7.8	89
229	Interference-free analysis using three-way fluorescence data and the parallel factor model. Determination of fluoroquinolone antibiotics in human serum. <i>Analytical Chemistry</i> , <b>2003</b> , 75, 2640-6	7.8	88
228	A new and efficient variable selection algorithm based on ant colony optimization. Applications to near infrared spectroscopy/partial least-squares analysis. <i>Analytica Chimica Acta</i> , <b>2011</b> , 699, 18-25	6.6	86
227	Trilinear least-squares and unfolded-PLS coupled to residual trilinearization: New chemometric tools for the analysis of four-way instrumental data. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2006</b> , 80, 77-86	3.8	82
226	Simultaneous spectrophotometric-multivariate calibration determination of several components of ophthalmic solutions: phenylephrine, chloramphenicol, antipyrine, methylparaben and thimerosal. <i>Talanta</i> , <b>2000</b> , 52, 909-20	6.2	82
225	Substituent and solvent effects on the proton transfer equilibrium in anils and azo derivatives of naphthol. Multinuclear NMR study and theoretical calculations. <i>Journal of Molecular Structure</i> , <b>2004</b> , 705, 1-9	3.4	77
224	A review on second- and third-order multivariate calibration applied to chromatographic data. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , <b>2012</b> , 910, 22-30 <sup>3-2</sup>		75
223	A review of multivariate calibration methods applied to biomedical analysis. <i>Microchemical Journal</i> , <b>2006</b> , 82, 29-42	4.8	73
222	A closed-form expression for computing the sensitivity in second-order bilinear calibration. <i>Journal of Chemometrics</i> , <b>2005</b> , 19, 583-592	1.6	68
221	Standard error of prediction in parallel factor analysis of three-way data. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2004</b> , 70, 75-82	3.8	65
220	Determination of five pesticides in juice, fruit and vegetable samples by means of liquid chromatography combined with multivariate curve resolution. <i>Analytica Chimica Acta</i> , <b>2014</b> , 814, 23-30	6.6	63
219	Second-order advantage achieved by unfolded-partial least-squares/residual bilinearization modeling of excitation-emission fluorescence data presenting inner filter effects. <i>Analytical Chemistry</i> , <b>2006</b> , 78, 8051-8	7.8	63
218	Different strategies for the direct determination of amoxicillin in human urine by second-order multivariate analysis of kinetic-spectrophotometric data. <i>Talanta</i> , <b>2007</b> , 71, 806-15	6.2	62
217	Simultaneous determination of rifampicin, isoniazid and pyrazinamide in tablet preparations by multivariate spectrophotometric calibration. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>1999</b> , 20, 681-6	3.5	61
216	Development of a novel strategy for preconcentration of antibiotic residues in milk and their quantitation by capillary electrophoresis. <i>Talanta</i> , <b>2010</b> , 82, 213-21	6.2	59
215	Visible/near infrared-partial least-squares analysis of Brix in sugar cane juice. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2010</b> , 102, 100-109	3.8	59
214	A test field for the second-order advantage in bilinear least-squares and parallel factor analyses: fluorescence determination of ciprofloxacin in human urine. <i>Analytical Chemistry</i> , <b>2004</b> , 76, 2798-806	7.8	59
213	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). <i>Analyst</i> , <b>1999</b> , 124, 725-731	5	58

212	13 C NMR spectroscopic and AM1 study of the intramolecular proton transfer in anils of salicylaldehyde and 2-hydroxynaphthalene-1-carbaldehyde. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1994</b> , 1067-1070		56
211	Development of novel formulations for Chagas disease: Optimization of benzimidazole chitosan microparticles based on artificial neural networks. <i>International Journal of Pharmaceutics</i> , <b>2009</b> , 367, 140-7	6.5	55
210	Simultaneous determination of levodopa and benserazide by stopped-flow injection analysis and three-way multivariate calibration of kinetic-spectrophotometric data. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>2004</b> , 36, 541-7	3.5	54
209	Wavelength selection for multivariate calibration using a genetic algorithm: a novel initialization strategy. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2002</b> , 42, 1146-53		54
208	Spectrofluorometric determination of diclofenac in tablets and ointments. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>1999</b> , 20, 587-90	3.5	54
207	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. <i>Journal of the American Chemical Society</i> , <b>1992</b> , 114, 5758-5763	16.4	54
206	New developments for the sensitivity estimation in four-way calibration with the quadrilinear parallel factor model. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 186-93	7.8	53
205	Multivariate partial least-squares coupled to residual trilinearization: a genuine multidimensional tool for the study of third-order data. Simultaneous analysis of procaine and its metabolite p-aminobenzoic acid in equine serum. <i>Analytical Chemistry</i> , <b>2007</b> , 79, 6949-58	7.8	53
204	Evaluation of partial least-squares with second-order advantage for the multi-way spectroscopic analysis of complex biological samples in the presence of analyte-background interactions. <i>Analyst, The</i> , <b>2006</b> , 131, 718-23	5	53
203	A new family of genetic algorithms for wavelength interval selection in multivariate analytical spectroscopy. <i>Journal of Chemometrics</i> , <b>2003</b> , 17, 338-345	1.6	52
202	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. <i>Analyst, The</i> , <b>2010</b> , 135, 636-42	5	51
201	First- and second-order multivariate calibration applied to biological samples: determination of anti-inflammatories in serum and urine. <i>Analytical and Bioanalytical Chemistry</i> , <b>2002</b> , 374, 451-9	4.4	51
200	Recent advances in analytical calibration with multi-way data. <i>Analytical Methods</i> , <b>2012</b> , 4, 1876	3.2	50
199	Tautomerism of representative aromatic hydroxy carbaldehyde anils as studied by spectroscopic methods and AM1 calculations. Synthesis of 10-hydroxyphenanthrene-9-carbaldehyde. <i>Tetrahedron</i> , <b>1995</b> , 51, 4619-4626	2.4	50
198	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. <i>Talanta</i> , <b>2013</b> , 103, 361-70	6.2	47
197	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. <i>Talanta</i> , <b>2009</b> , 77, 1715-23	6.2	47
196	New robust bilinear least squares method for the analysis of spectral-pH matrix data. <i>Applied Spectroscopy</i> , <b>2005</b> , 59, 926-33	3.1	47
195	High-resolution solid-state carbon-13 NMR spectra of porphine and 5,10,15,20-tetraalkylporphyrins: implications for the nitrogen-hydrogen tautomerization process. <i>Journal of the American Chemical Society</i> , <b>1988</b> , 110, 336-342	16.4	47

194	MVC3: A MATLAB graphical interface toolbox for third-order multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2012</b> , 116, 9-16	3.8	46
193	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 interferences. <i>Analytica Chimica Acta</i> , <b>2010</b> , 677, 97-107	6.6	46
192	Multi-way chromatographic calibration-A review. <i>Journal of Chromatography A</i> , <b>2019</b> , 1587, 2-13	4.5	43
191	Second-order advantage from kinetic-spectroscopic data matrices in the presence of extreme spectral overlapping A multivariate curve resolution--alternating least-squares approach. <i>Analytica Chimica Acta</i> , <b>2008</b> , 614, 46-57	6.6	42
190	Chemometric processing of second-order liquid chromatographic data with UV-vis and fluorescence detection. A comparison of multivariate curve resolution and parallel factor analysis 2. <i>Analytica Chimica Acta</i> , <b>2014</b> , 842, 11-9	6.6	41
189	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. <i>Journal of Agricultural and Food Chemistry</i> , <b>2004</b> , 52, 2479-84	5.7	41
188	Two multivariate strategies applied to three-way kinetic spectrophotometric data for the determination of mixtures of the pesticides carbaryl and chlorpyrifos. <i>Applied Spectroscopy</i> , <b>2004</b> , 58, 83-90	3.1	41
187	Phenolic profiling of grapes, fermenting samples and wines using UV-Visible spectroscopy with chemometrics. <i>Food Control</i> , <b>2018</b> , 85, 11-22	6.2	40
186	Determination of pesticides and metabolites in wine by high performance liquid chromatography and second-order calibration methods. <i>Journal of Chromatography A</i> , <b>2007</b> , 1148, 200-10	4.5	40
185	Four-way data coupled to parallel factor model applied to environmental analysis: determination of 2,3,7,8-tetrachloro-dibenzo-para-dioxin in highly contaminated waters by solid-liquid extraction laser-excited time-resolved Shpol'skii spectroscopy. <i>Analytical Chemistry</i> , <b>2005</b> , 77, 2608-16	7.8	40
184	Anthocyanins as markers for the classification of Argentinean wines according to botanical and geographical origin. Chemometric modeling of liquid chromatography-mass spectrometry data. <i>Food Chemistry</i> , <b>2015</b> , 175, 174-80	8.5	39
183	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. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2011</b> , 100, 170-187	3.8	39
182	Nonlinear four-way kinetic-excitation-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. <i>Analytical Chemistry</i> , <b>2008</b> , 80, 7248-56	7.8	39
181	Determination of theophylline in blood serum by UV spectrophotometry and partial least-squares (PLS-1) calibration. <i>Analytica Chimica Acta</i> , <b>1999</b> , 384, 95-103	6.6	38
180	Simultaneous determination of phenobarbital and phenytoin in tablet preparations by multivariate spectrophotometric calibration. <i>Talanta</i> , <b>1998</b> , 47, 103-8	6.2	37
179	Screening of oil samples on the basis of excitation-emission room-temperature phosphorescence data and multiway chemometric techniques. Introducing the second-order advantage in a classification study. <i>Analytical Chemistry</i> , <b>2008</b> , 80, 2789-98	7.8	37
178	Sustained prediction ability of net analyte preprocessing methods using reduced calibration sets. Theoretical and experimental study involving the spectrophotometric analysis of multicomponent mixtures. <i>Analyst</i> , <b>2001</b> , 126, 1105-12	5	37
177	Chemometrics coupled to vibrational spectroscopy and spectroscopic imaging for the analysis of solid-phase pharmaceutical products: A brief review on non-destructive analytical methods. <i>TrAC - Trends in Analytical Chemistry</i> , <b>2018</b> , 108, 74-87	14.6	37

176	Chemometric assisted simultaneous spectrophotometric determination of four-component nasal solutions with a reduced number of calibration samples. <i>Analytica Chimica Acta</i> , <b>2002</b> , 453, 289-300	6.6	36
175	Solid-state electronic absorption, fluorescence and <sup>13</sup> C CPMAS NMR spectroscopic study of thermo- and photo-chromic aromatic Schiff bases. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1996</b> , 2293-2296		36
174	Microcomputer simulation of solid-state <sup>13</sup> C NMR line shapes affected by quadrupolar nuclei. <i>Magnetic Resonance in Chemistry</i> , <b>1988</b> , 26, 615-618	2.1	36
173	Three-way partial least-squares/residual bilinearization study of second-order lanthanide-sensitized luminescence excitation-time decay data: analysis of benzoic acid in beverage samples. <i>Analytica Chimica Acta</i> , <b>2008</b> , 610, 186-95	6.6	35
172	A variable-temperature solid-state carbon-13 CPMAS NMR analysis of meso-tetrapropylporphyrin and of octaethylporphyrin. <i>Journal of the American Chemical Society</i> , <b>1988</b> , 110, 5651-5661	16.4	35
171	Comparative chemometric analysis of fluorescence and near infrared spectroscopies for authenticity confirmation and geographical origin of Argentinean extra virgin olive oils. <i>Food Control</i> , <b>2019</b> , 96, 22-28	6.2	34
170	Direct and simultaneous spectrofluorometric determination of naproxen and salicylate in human serum assisted by chemometric analysis. <i>Analytica Chimica Acta</i> , <b>2002</b> , 471, 87-96	6.6	34
169	Analytical figures of merit for partial least-squares coupled to residual multilinearization. <i>Analytical Chemistry</i> , <b>2012</b> , 84, 10823-30	7.8	33
168	A road map for multi-way calibration models. <i>Analyst, The</i> , <b>2017</b> , 142, 2862-2873	5	32
167	Evaluation of complex spectral-pH three-way arrays by modified bilinear least-squares: determination of four different dyes in interfering systems. <i>Analyst, The</i> , <b>2005</b> , 130, 1291-8	5	32
166	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. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2008</b> , 92, 61-70	3.8	31
165	In vivo evaluation of albendazole microspheres for the treatment of <i>Toxocara canis</i> larva migrans. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , <b>2010</b> , 75, 451-4	5.7	30
164	A novel second-order standard addition analytical method based on data processing with multidimensional partial least-squares and residual bilinearization. <i>Analytica Chimica Acta</i> , <b>2009</b> , 651, 165-72	6.6	30
163	Flow injection system for the on-line preconcentration of Pb by cloud point extraction coupled to USNIP OES. <i>Microchemical Journal</i> , <b>2010</b> , 95, 306-310	4.8	30
162	Complementary use of partial least-squares and artificial neural networks for the non-linear spectrophotometric analysis of pharmaceutical samples. <i>Analytical and Bioanalytical Chemistry</i> , <b>2002</b> , 374, 460-5	4.4	30
161	Quadrupole effects of spin-3/2 nuclei on the solid-state magic-angle spinning nuclear magnetic resonance spectra of spin-1/2 nuclei. Deviations from first-order theory and implications concerning the sign of the indirect coupling constant. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1993</b> , 2, 325-34	3.1	30
160	A simple approach to uncertainty propagation in preprocessed multivariate calibration. <i>Journal of Chemometrics</i> , <b>2002</b> , 16, 207-217	1.6	29
159	Design and optimization of a chemometrics-assisted spectrophotometric method for the simultaneous determination of levodopa and carbidopa in pharmaceutical products. <i>Analytica Chimica Acta</i> , <b>2005</b> , 543, 192-198	6.6	29

158	Concerning the crystal structure of porphine: a proton pulsed and carbon-13 cross-polarization/magic-angle-spinning NMR study. <i>Journal of the American Chemical Society</i> , <b>1989</b> , 111, 7001-7005	16.4	29
157	Analysis of amoxicillin in human urine by photo-activated generation of fluorescence excitation-emission matrices and artificial neural networks combined with residual bilinearization. <i>Analytica Chimica Acta</i> , <b>2007</b> , 588, 192-9	6.6	28
156	Development and validation of chemometrics-assisted spectrophotometry and micellar electrokinetic chromatography for the determination of four-component pharmaceuticals. <i>Analytica Chimica Acta</i> , <b>2003</b> , 489, 77-84	6.6	28
155	Second-order analyte quantitation under identical profiles in one data dimension. A dependency-adapted partial least-squares/residual bilinearization method. <i>Analytical Chemistry</i> , <b>2010</b> , 82, 4510-9	7.8	27
154	Chemometrics assisted spectroscopic determination of vitamin B6, vitamin B12 and dexamethasone in injectables. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>2003</b> , 31, 621-7	3.5	27
153	The effects of interplay between quadrupolar, dipolar and shielding tensors on magic-angle spinning NMR spectra: shapes of spinning sidebands. <i>Molecular Physics</i> , <b>1996</b> , 87, 669-677	1.7	27
152	Multiple response optimization of styrene-butadiene rubber emulsion polymerization. <i>Computers and Chemical Engineering</i> , <b>2009</b> , 33, 850-856	4	26
151	Chemometric resolution of fully overlapped CE peaks: quantitation of carbamazepine in human serum in the presence of several interferences. <i>Electrophoresis</i> , <b>2008</b> , 29, 4527-37	3.6	26
150	Solid-liquid Extraction Room Temperature Phosphorimetry and Pattern Recognition for Screening Polycyclic Aromatic Hydrocarbons and Polychlorinated Biphenyls in Water Samples. <i>Environmental Science &amp; Technology</i> , <b>2003</b> , 37, 1385-1391	10.3	26
149	A combined artificial neural network/residual bilinearization approach for obtaining the second-order advantage from three-way non-linear data. <i>Journal of Chemometrics</i> , <b>2005</b> , 19, 615-624	1.6	26
148	A new modeling strategy for third-order fast high-performance liquid chromatographic data with fluorescence detection. Quantitation of fluoroquinolones in water samples. <i>Analytical and Bioanalytical Chemistry</i> , <b>2015</b> , 407, 1999-2011	4.4	25
147	Simultaneous multivariate spectrophotometric analysis of paracetamol and minor components (diphenhydramine or phenylpropanolamine) in tablet preparations. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>1999</b> , 20, 255-61	3.5	25
146	The effect of data matrix augmentation and constraints in extended multivariate curve resolution-alternating least squares. <i>Journal of Chemometrics</i> , <b>2017</b> , 31, e2875	1.6	24
145	Introduction to Multivariate Calibration <b>2018</b> ,		24
144	Quantifying the Prediction Error in Analytical Multivariate Curve Resolution Studies of Multicomponent Systems. <i>Analytical Chemistry</i> , <b>2018</b> , 90, 7040-7047	7.8	23
143	Spectroscopic and potentiometric study of aromatic-hydroxy azo compounds and their copper(II)complexes. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1997</b> , 93, 545-551		23
142	Analytical chemistry assisted by multi-way calibration: A contribution to green chemistry. <i>Talanta</i> , <b>2019</b> , 204, 700-712	6.2	22
141	Spray drying formulation of albendazole microspheres by experimental design. In vitro-in vivo studies. <i>Drug Development and Industrial Pharmacy</i> , <b>2015</b> , 41, 244-52	3.6	22

140	Generalized error-dependent prediction uncertainty in multivariate calibration. <i>Analytica Chimica Acta</i> , <b>2016</b> , 903, 51-60	6.6	22
139	Structural analysis of natural deep eutectic solvents. Theoretical and experimental study. <i>Microchemical Journal</i> , <b>2018</b> , 143, 252-258	4.8	22
138	An integrated approach to the simultaneous selection of variables, mathematical pre-processing and calibration samples in partial least-squares multivariate calibration. <i>Talanta</i> , <b>2013</b> , 115, 755-60	6.2	22
137	When unfolding is better: unique success of unfolded partial least-squares regression with residual bilinearization for the processing of spectral-pH data with strong spectral overlapping. Analysis of fluoroquinolones in human urine based on flow-injection pH-modulated synchronous fluorescence data matrices. <i>Analyst, The</i> , <b>2009</b> , 134, 1682-91	5	22
136	Fast spectrophotometric determination of fluoride in ground waters by flow injection using partial least-squares calibration. <i>Analytica Chimica Acta</i> , <b>2004</b> , 512, 157-163	6.6	22
135	Rigorous Statistical Analysis of Errors in Chemical-Shift-Tensor Components Obtained from Spinning Sidebands in Solid-State NMR. <i>Journal of Magnetic Resonance Series A</i> , <b>1996</b> , 123, 207-210		22
134	Novel augmented parallel factor model for four-way calibration of high-performance liquid chromatography fluorescence excitation-emission data. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2015</b> , 141, 1-11	3.8	21
133	Multivariate curve-resolution analysis of pesticides in water samples from liquid chromatographic-diode array data. <i>Talanta</i> , <b>2011</b> , 83, 1173-80	6.2	21
132	Multiresponse optimization of the properties of albendazole-chitosan microparticles. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>2008</b> , 48, 802-7	3.5	21
131	Spectroscopic bilinear least-squares methods exploiting the second-order advantage. Theoretical and experimental study concerning accuracy, sensitivity and prediction error. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2006</b> , 80, 99-108	3.8	21
130	Simultaneous Multivariate Spectrophotometric Analysis of Binary and Ternary Mixtures of Sulfamethoxazole, Trimethoprim and Phenazopyridine in Tablets. <i>Analytical Letters</i> , <b>1999</b> , 32, 1389-1401 <sup>2.2</sup>		21
129	Ground- and excited-state prototropic tautomerism in anils of aromatic hydroxy aldehydes studied by electronic absorption, fluorescence and <sup>1</sup> H and <sup>13</sup> C NMR spectroscopies and semi-empirical calculations. <i>Journal of Physical Organic Chemistry</i> , <b>1995</b> , 8, 713-720	2.1	21
128	Sensitivity, Prediction Uncertainty, and Detection Limit for Artificial Neural Network Calibrations. <i>Analytical Chemistry</i> , <b>2016</b> , 88, 7807-12	7.8	20
127	Determination of tributyltin at parts-per-trillion levels in natural waters by second-order multivariate calibration and fluorescence spectroscopy. <i>Microchemical Journal</i> , <b>2013</b> , 106, 95-101	4.8	20
126	Time dependence of the aroma pattern emitted by an encapsulated essence studied by means of electronic noses and chemometric analysis. <i>Food Research International</i> , <b>2010</b> , 43, 797-804	7	20
125	Spectrofluorimetric determination of phenylephrine in the presence of a large excess of paracetamol. <i>Analytica Chimica Acta</i> , <b>2000</b> , 419, 159-168	6.6	20
124	A multiway approach for classification and characterization of rabbit liver apothioneins by CE-ESI-MS. <i>Electrophoresis</i> , <b>2008</b> , 29, 4355-67	3.6	19
123	Experimental study of non-linear second-order analytical data with focus on the second-order advantage. <i>Analyst, The</i> , <b>2007</b> , 132, 654-63	5	19

122	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. <i>Analytica Chimica Acta</i> , <b>2005</b> , 553, 141-147	6.6	19
121	Simultaneous Determination of Timolol Maleate and Pilocarpine Hydrochloride in Ophthalmic Solutions by First Derivative UV Spectrophotometry and PLS-1 Multivariate Calibration. <i>Analytical Letters</i> , <b>1999</b> , 32, 2019-2033	2.2	19
120	A simple theoretical treatment of quadrupolar effects on magic-angle-spinning solid-state NMR spectra of spin-1/2 nuclei in the limit of large quadrupole coupling constants. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1993</b> , 1, 345-53	3.1	19
119	<sup>13</sup> C CPMAS NMR study of solid arylazonaphthols. Evidence of <sup>13</sup> C, <sup>14</sup> N self-decoupling induced by a solid-state proton transfer reaction. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1993</b> , 1783-1786		18
118	Classification of olive oils according to their cultivars based on second-order data using LC-DAD. <i>Talanta</i> , <b>2019</b> , 195, 69-76	6.2	18
117	MVC3_GUI: A MATLAB graphical user interface for third-order multivariate calibration. An upgrade including new multi-way models. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2018</b> , 173, 21-29	3.8	17
116	Ground and excited state proton transfer in intramolecularly hydrogen bonded aromatic hydroxy azo, aldehydes and their derivatives. <i>Journal of Molecular Structure</i> , <b>1997</b> , 415, 115-121	3.4	16
115	Simultaneous spectrofluorometric determination of oxatomide and phenylephrine in the presence of a large excess of paracetamol. <i>Analytica Chimica Acta</i> , <b>2001</b> , 439, 87-94	6.6	16
114	Determination of three aspirin metabolites in human urine by derivative synchronous spectrofluorimetry. <i>Analyst, The</i> , <b>1995</b> , 120, 443-445	5	16
113	A new and consistent parameter for measuring the quality of multivariate analytical methods: Generalized analytical sensitivity. <i>Analytica Chimica Acta</i> , <b>2016</b> , 933, 43-9	6.6	15
112	Residual bilinearization combined with kernel-unfolded partial least-squares: A new technique for processing non-linear second-order data achieving the second-order advantage. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2010</b> , 100, 127-135	3.8	15
111	Simultaneous multiresponse optimization applied to epinastine determination in human serum by using capillary electrophoresis. <i>Analytica Chimica Acta</i> , <b>2007</b> , 595, 310-8	6.6	15
110	Sample-specific standard prediction errors in three-way parallel factor analysis (PARAFAC) exploiting the second-order advantage. <i>Journal of Chemometrics</i> , <b>2004</b> , 18, 363-371	1.6	15
109	Artificial neural networks study of the catalytic reduction of resazurin: stopped-flow injection kinetic-spectrophotometric determination of Cu(II) and Ni(II). <i>Analytica Chimica Acta</i> , <b>2005</b> , 528, 275-284	6.6	15
108	Residual Dipolar ( <sup>35</sup> Cl, <sup>13</sup> C) Coupling in Solid Sodium Chloroacetates. A Combined Variable-Temperature <sup>35</sup> Cl NQR and Variable-Field <sup>13</sup> C MAS NMR Study. <i>Journal of Magnetic Resonance Series A</i> , <b>1995</b> , 116, 244-250		15
107	Interpretation of matrix chromatographic-spectral data modeling with parallel factor analysis 2 and multivariate curve resolution. <i>Journal of Chromatography A</i> , <b>2019</b> , 1604, 460502	4.5	14
106	SIMULTANEOUS MULTIVARIATE SPECTROPHOTOMETRIC ANALYSIS OF EAR DROPS CONTAINING A TERNARY MIXTURE OF ANTIPYRINE, SULFATHIAZOLE, AND RIVANOL. <i>Analytical Letters</i> , <b>2001</b> , 34, 2077-2088	2.2	14
105	Determination of the Active Principle in a Syrup by Spectrophotometry and Principal Component Regression Analysis. An Advanced Undergraduate Experiment Involving Chemometrics. <i>Journal of Chemical Education</i> , <b>2000</b> , 77, 1330	2.4	14

104	A <sup>13</sup> C solid-state NMR study of the structure and the dynamics of the polymorphs of sulphanilamide. <i>Molecular Physics</i> , <b>1990</b> , 70, 563-579	1.7	14
103	A systematic study on the effect of noise and shift on multivariate figures of merit of second-order calibration algorithms. <i>Analytica Chimica Acta</i> , <b>2017</b> , 952, 18-31	6.6	13
102	A New Genetic Algorithm Applied to the near Infrared Analysis of Gasolines. <i>Journal of Near Infrared Spectroscopy</i> , <b>2004</b> , 12, 85-91	1.5	13
101	Net Analyte Preprocessing: A New and Versatile Multivariate Calibration Technique. Analysis of Mixtures of Rubber Antioxidants by NIR Spectroscopy. <i>Journal of Near Infrared Spectroscopy</i> , <b>2001</b> , 9, 245-254	1.5	13
100	C,O atomic motion associated with solid-state proton transfer in enolic 1,3-diketones. <i>Journal of Molecular Structure</i> , <b>1992</b> , 274, 215-222	3.4	13
99	Stereoselective synthesis of the novel bisnorditerpene grindelstrictic acid, isolated from <i>Grindelia stricta</i> . <i>Journal of Organic Chemistry</i> , <b>1986</b> , 51, 2824-2826	4.2	13
98	Processing multi-way chromatographic data for analytical calibration, classification and discrimination: A successful marriage between separation science and chemometrics. <i>TrAC - Trends in Analytical Chemistry</i> , <b>2021</b> , 134, 116128	14.6	13
97	Strategy To Obtain Accurate Analytical Solutions in Second-Order Multivariate Calibration with Curve Resolution Methods. <i>Analytical Chemistry</i> , <b>2018</b> , 90, 9725-9733	7.8	12
96	Urea-phosphoric acid complex studied by variable temperature <sup>31</sup> P NMR spectroscopy and semiempirical calculations. <i>Journal of Physics and Chemistry of Solids</i> , <b>1996</b> , 57, 1183-1190	3.9	12
95	Total Fluorescence and Zero-Crossing First-Derivative Synchronous Fluorescence Determination Of Acetylsalicylic Acid Metabolites in Biological Fluids. <i>Analytical Letters</i> , <b>1993</b> , 26, 247-257	2.2	12
94	Solid State NMR of Drugs: Soluble Aspirin. <i>Analytical Letters</i> , <b>1987</b> , 20, 1657-1666	2.2	12
93	Why should the pharmaceutical industry claim for the implementation of second-order chemometric models-A critical review. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>2020</b> , 179, 112965	2.5	12
92	Design, characterization, and in vitro evaluation of antifungal polymeric films. <i>AAPS PharmSciTech</i> , <b>2013</b> , 14, 64-73	3.9	11
91	Near-infrared spectroscopic determination of antioxidants and organic acids in rubbers assisted by a new multivariate calibration method based on direct orthogonalization. <i>Analyst, The</i> , <b>2002</b> , 127, 304-309	5	11
90	Determination of the minor component bromhexine in cotrimoxazole-containing tablets by absorption spectrophotometry and partial least-squares (PLS-1) multivariate calibration. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>2000</b> , 23, 591-5	3.5	11
89	Second-order quadrupolar effects for directly bonded and remote <sup>13</sup> C/ <sup>79</sup> /81Br spin pairs in high-resolution <sup>13</sup> C NMR spectra of solids. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1995</b> , 91, 3167-3176		11
88	Sensitivity for Multivariate Calibration Based on Multilayer Perceptron Artificial Neural Networks. <i>Analytical Chemistry</i> , <b>2020</b> , 92, 12265-12272	7.8	11
87	Improvement of residual bilinearization by particle swarm optimization for achieving the second-order advantage with unfolded partial least-squares. <i>Journal of Chemometrics</i> , <b>2007</b> , 21, 557-566	1.6	10

86	Estimation of the composition of recombinant human erythropoietin mixtures using capillary electrophoresis and multivariate calibration methods. <i>Electrophoresis</i> , <b>2006</b> , 27, 4008-15	3.6	10
85	Deuterium isotope effects on <sup>31</sup> P NMR parameters: hydrogen bonding in a solid urea-phosphoric acid adduct. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1996</b> , 92, 5047-5050		10
84	Stereospecific transformation of grindelic acid into the antifeedant 6.alpha.-hydroxygrindelic acid, its 6.beta.-epimer, and other related natural diterpene acids. <i>Journal of Organic Chemistry</i> , <b>1984</b> , 49, 4984-4988 <sup>10</sup>	4.2	10
83	Chemometric modeling of kinetic-fluorescent third-order data for thiamine determination in multivitamin complexes. <i>Microchemical Journal</i> , <b>2016</b> , 128, 42-46	4.8	10
82	SRO_ANN: An integrated MatLab toolbox for multiple surface response optimization using radial basis functions. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2017</b> , 171, 198-206	3.8	9
81	Uncovering interactions in Plackett-Burman screening designs applied to analytical systems. A Monte Carlo ant colony optimization approach. <i>Talanta</i> , <b>2012</b> , 97, 242-8	6.2	9
80	Principal component analysis-adaptive neuro-fuzzy inference systems (ANFISs) for the simultaneous spectrophotometric determination of three metals in water samples. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2009</b> , 73, 608-14	4.4	9
79	Random Error Analysis in the Determination of Equilibrium Constants of Very Stable Metal Complexes.. <i>Analytical Letters</i> , <b>1997</b> , 30, 1967-1980	2.2	9
78	Magic-angle-spinning <sup>31</sup> P NMR spectra of solid dihydrogen phosphates. Comparison of ordered and dynamically disordered compounds. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1992</b> , 1, 205-10	3.1	9
77	Structural and <sup>14</sup> N EFG Information on Solid Imidazole by <sup>13</sup> C CP/MAS NMR Data. <i>Spectroscopy Letters</i> , <b>1991</b> , 24, 895-907	1.1	9
76	Recent advances in analytical figures of merit: heteroscedasticity strikes back. <i>Analytical Methods</i> , <b>2017</b> , 9, 739-743	3.2	8
75	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2014</b> , 122, 721-30	4.4	8
74	Optimization of the hydrolysis of lignocellulosic residues by using radial basis functions modeling and particle swarm optimization. <i>Biochemical Engineering Journal</i> , <b>2013</b> , 80, 1-9	4.2	8
73	Determination of enantiomeric composition of ibuprofen in pharmaceutical formulations by partial least-squares regression of strongly overlapped chromatographic profiles. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , <b>2012</b> , 910, 78-83	3.2	8
72	SIMULTANEOUS DETERMINATION OF NICOTINAMIDE AND INOSINE IN OPHTHALMIC SOLUTIONS BY UV SPECTROPHOTOMETRY AND PLS-1 MULTIVARIATE CALIBRATION. <i>Analytical Letters</i> , <b>2001</b> , 34, 363-376	2.2	8
71	Multivariate Calibration: A Powerful Tool in Pharmaceutical Analysis. <i>Current Pharmaceutical Analysis</i> , <b>2005</b> , 1, 145-154	0.6	8
70	Multi-way figures of merit in the presence of heteroscedastic and correlated instrumental noise: Unfolded partial least-squares with residual multi-linearization. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2016</b> , 158, 200-209	3.8	8
69	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. <i>Journal of Chemometrics</i> , <b>2020</b> , 34, e3130	1.6	8

68	A novel application of nylon membranes for tributyltin determination in complex environmental samples by fluorescence spectroscopy and multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2015</b> , 148, 77-84	3.8	7
67	A New Parameter for Measuring the Prediction Uncertainty Produced by Rotational Ambiguity in Second-Order Calibration with Multivariate Curve Resolution. <i>Analytical Chemistry</i> , <b>2020</b> , 92, 9118-9123	7.8	7
66	Recent applications of first- and second-order multivariate calibration to analytical chemistry. <i>Journal of AOAC INTERNATIONAL</i> , <b>2014</b> , 97, 39-49	1.7	7
65	Solid state NMR sideband shape simulations for any spinning angle and speed. First order calculation of residual dipolar coupling to quadrupolar nuclei. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1997</b> , 10, 19-24	3.1	7
64	EPSILON: a versatile microcomputer program for the spectrophotometric data analysis of metal-ligand equilibria. <i>Computers &amp; Chemistry</i> , <b>1998</b> , 22, 161-168		7
63	Rapid Determination of Paracetamol in Blood Serum Samples by First-Derivative UV Absorption Spectroscopy. <i>Analytical Letters</i> , <b>1995</b> , 28, 2219-2226	2.2	7
62	Solution of acid-base equilibria by successive approximations. <i>Journal of Chemical Education</i> , <b>1990</b> , 67, 229	2.4	7
61	On second-order calibration based on multivariate curve resolution in the presence of highly overlapped profiles. <i>Analytica Chimica Acta</i> , <b>2020</b> , 1096, 53-60	6.6	7
60	A down-to-earth analyst view of rotational ambiguity in second-order calibration with multivariate curve resolution—a tutorial. <i>Analytica Chimica Acta</i> , <b>2021</b> , 1156, 338206	6.6	7
59	Online Third-Order Liquid Chromatographic Data with Native and Photoinduced Fluorescence Detection for the Quantitation of Organic Pollutants in Environmental Water. <i>ACS Omega</i> , <b>2018</b> , 3, 15773-15779	3.9	7
58	Initialization effects in two-component second-order multivariate calibration with the extended bilinear model. <i>Analytica Chimica Acta</i> , <b>2020</b> , 1125, 169-176	6.6	6
57	Error Covariance Penalized Regression: A novel multivariate model combining penalized regression with multivariate error structure. <i>Analytica Chimica Acta</i> , <b>2018</b> , 1011, 20-27	6.6	6
56	The effect of constraints on the analytical figures of merit achieved by extended multivariate curve resolution-alternating least-squares. <i>Analytica Chimica Acta</i> , <b>2018</b> , 1003, 10-15	6.6	6
55	Chemometric modeling of organic contaminant sources in surface waters of a mediterranean river basin. <i>Environmental Sciences: Processes and Impacts</i> , <b>2014</b> , 16, 124-34	4.3	6
54	Unfolded and Multiway Partial Least-Squares with Residual Multilinearization. <i>Data Handling in Science and Technology</i> , <b>2015</b> , 29, 365-397	2.7	6
53	Figures of Merit in Multiway Calibration. <i>Data Handling in Science and Technology</i> , <b>2015</b> , 29, 541-575	2.7	6
52	Teaching Chemometrics with a Bioprocess: Analytical Methods Comparison Using Bivariate Linear Regression. <i>The Chemical Educator</i> , <b>2002</b> , 7, 265-269		6
51	An extension of the Beierbeck and Saunders parameters for the semiempirical calculation of the <sup>13</sup> C nuclear magnetic resonance chemical shifts: the gauche-(X) effect in epoxides. <i>Canadian Journal of Chemistry</i> , <b>1986</b> , 64, 552-555	0.9	6

50	MVC1_GUI: A MATLAB graphical user interface for first-order multivariate calibration. An upgrade including artificial neural networks modelling. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2020</b> , 206, 104162	3.8	6
49	Multivariate curve resolution applied to kinetic-spectroscopic data matrices: Dye determination in foods by means of enzymatic oxidation. <i>Talanta</i> , <b>2017</b> , 169, 189-194	6.2	5
48	Proton transfer and Cu(II) binuclear complexes of 1,4-bis-p-sulfonylazo-2,3-dihydroxynaphthalene: a spectroscopic and potentiometric study in aqueous solution. <i>Journal of Molecular Structure</i> , <b>1997</b> , 435, 199-206	3.4	5
47	Conformational analysis of the 4a-methyl octahydrophenanthrene system. A spectroscopic and theoretical approach. <i>Tetrahedron</i> , <b>1989</b> , 45, 4951-4960	2.4	5
46	Calculation of solubilities of carbonates and phosphates in water as influenced by competitive acid-base reactions. <i>Journal of Chemical Education</i> , <b>1990</b> , 67, 934	2.4	5
45	Semiempirical calculation of <sup>13</sup> C nuclear magnetic resonance chemical shifts of acyclic hydrocarbons. Application to the stereochemical analysis of steroidal side chains. <i>Canadian Journal of Chemistry</i> , <b>1988</b> , 66, 71-75	0.9	5
44	N-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. <i>Journal of Chemometrics</i> , <b>2021</b> , 35, e3317	1.6	5
43	Contribution to second-order calibration based on multivariate curve resolution with and without previous chromatographic synchronization. <i>Analytica Chimica Acta</i> , <b>2019</b> , 1078, 8-15	6.6	4
42	Complex numbers-partial least-squares applied to the treatment of electrochemical impedance spectroscopy data. <i>Analytica Chimica Acta</i> , <b>2019</b> , 1080, 1-11	6.6	4
41	Calibration Scenarios <b>2014</b> , 1-9		4
40	Unfolded and Multiway Partial Least-Squares with Residual Multilinearization: Fundamentals. <i>Data Handling in Science and Technology</i> , <b>2015</b> , 29, 347-363	2.7	4
39	Partial Least-Squares with Residual Bilinearization <b>2014</b> , 157-195		4
38	Retrieving <sup>31</sup> P Chemical-Shift-Tensor Information for Dihydrogen Phosphates in the Presence of Homonuclear <sup>31</sup> P- <sup>31</sup> P Dipolar Coupling. <i>Journal of Magnetic Resonance</i> , <b>1997</b> , 126, 138-41	3	4
37	<sup>13</sup> C CP/MAS NMR of a <sup>13</sup> C- <sup>2</sup> H residual dipolar coupled pair. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1996</b> , 7, 121-5	3.1	4
36	Zero-crossing first and second derivative synchronous fluorescence spectroscopic determination of aspirin metabolites in urine. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , <b>1994</b> , 12, 1333-5	3.5	4
35	Maximum likelihood unfolded principal component regression with residual bilinearization (MLU-PCR/RBL) for second-order multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2017</b> , 170, 51-57	3.8	3
34	Developing and Implementing an R Shiny Application to Introduce Multivariate Calibration to Advanced Undergraduate Students. <i>Journal of Chemical Education</i> , <b>2020</b> , 97, 1176-1180	2.4	3
33	Experimental Three-way/Second-order Data <b>2014</b> , 27-45		3

32	Simultaneous Determination of Two Antibiotics in Tablets by Spectrophotometry and Principal Component Regression (PCR) Analysis. An Advanced Undergraduate Experiment Involving Chemometrics. <i>The Chemical Educator</i> , <b>2000</b> , 5, 236-241		3
31	Retrieval of solid-state <sup>31</sup> P nuclear magnetic resonance (NMR) chemical shielding parameters: proposal of an approach concerning variable-temperature <sup>31</sup> P NMR mass spectra of urea phosphate and comparison of different methods. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1994</b> , 3, 163-70	3.1	3
30	<sup>14</sup> N Quadrupole Interactions in Nitrogen-Containing Ceramics. Effects on <sup>29</sup> Si NMR Line Shapes and Structural Implications. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>1992</b> , 47, 39-44	1.4	3
29	Model Studies For the Synthesis of Erigerol Synthesis of 1-Deoxy-13-Epigerol from Grindelic Acid. <i>Synthetic Communications</i> , <b>1987</b> , 17, 1727-1733	1.7	3
28	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. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2020</b> , 199, 103972	3.8	2
27	Chemometrics and Multivariate Calibration <b>2018</b> , 1-17		2
26	The Optimum Number of Latent Variables <b>2018</b> , 87-101		2
25	Analytical Figures of Merit <b>2014</b> , 93-107		2
24	Parallel Factor Analysis: Nontrilinear Data of Type 1 <b>2014</b> , 109-125		2
23	Illustrating rotating-frame ( <sup>1</sup> H)NMR relaxation with a microcomputer. <i>Concepts in Magnetic Resonance</i> , <b>1998</b> , 10, 157-166		2
22	Errors in chemical shift tensor components and orientation in the molecular frame as obtained from MAS NMR spinning sideband analysis. <i>Solid State Nuclear Magnetic Resonance</i> , <b>1998</b> , 11, 181-7	3.1	2
21	Determination of Equilibrium Constants of Metal Complexes from Spectrophotometric Measurements. An Undergraduate Laboratory Experiment. <i>Journal of Chemical Education</i> , <b>1999</b> , 76, 1277-4		2
20	A simple computer program for the calculation of <sup>13</sup> C-NMR chemical shifts. <i>Journal of Chemical Education</i> , <b>1989</b> , 66, 53	2.4	2
19	Microcomputer program based on the Beierbeck-Saunders approach for the prediction of <sup>13</sup> C-NMR chemical shifts in acyclic hydrocarbons. <i>Analytica Chimica Acta</i> , <b>1990</b> , 233, 315-319	6.6	2
18	Interference-free calibration with first-order instrumental data and multivariate curve resolution. When and why?. <i>Analytica Chimica Acta</i> , <b>2021</b> , 1161, 338465	6.6	2
17	Analytical Figures of Merit <b>2018</b> , 159-177		1
16	Mathematical Pre-processing <b>2018</b> , 139-158		1
15	Three-way/Second-order Standard Addition <b>2014</b> , 197-216		1

14	Spinning Sideband Analysis for Spin-1/2 Nuclei <b>2007</b> ,			1
13	Shifting of the keto-enol equilibrium in 1,3-diphenyl-1,3-propanedione by methyl substitution. An AM1 study. <i>Computational and Theoretical Chemistry</i> , <b>1994</b> , 309, 59-64			1
12	How noise affects the band boundaries in multivariate curve resolution. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2022</b> , 220, 104472	3.8		1
11	Sensitivity and generalized analytical sensitivity expressions for quantitative analysis using convolutional neural networks.. <i>Analytica Chimica Acta</i> , <b>2022</b> , 1192, 338697	6.6		1
10	Estimating the boundaries of the feasible profiles in the bilinear decomposition of multi-component data matrices. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2021</b> , 216, 104387	3.8		1
9	Achieving the analytical second-order advantage with non-bilinear second-order data. <i>Analytica Chimica Acta</i> , <b>2021</b> , 1181, 338911	6.6		0
8	Evaluation of the ambiguity in second-order analytical calibration based on multivariate curve resolution. A tutorial. <i>Microchemical Journal</i> , <b>2022</b> , 179, 107455	4.8		0
7	MVC1: Software for Multivariate Calibration <b>2018</b> , 179-205			
6	The Classical Least-Squares Model <b>2018</b> , 19-38			
5	The Partial Least-Squares Model <b>2018</b> , 103-121			
4	Third-order/Four-way Calibration and Beyond <b>2014</b> , 217-232			
3	On the signal contribution function with respect to different norms. <i>Journal of Chemometrics</i> , <b>2021</b> , 35, e3363	1.6		
2	Figures of Merit <b>2020</b> , 441-463			
1	Statistics and Food Quality <b>2021</b> , 362-386			