MarÃa Cruz Ortiz

List of Publications by Year
in descending order

126 papers	2,980 citations	172207 29 h-index	223531 46 g-index
126 all docs	126 docs citations	126 times ranked	2603 citing authors

#	Article	IF	Citations
1	Univariate data analysis versus multivariate approach in liquid chromatography. An application for melamine migration from food contact materials. Microchemical Journal, 2022, 181, 107648.	2.3	2
2	Procedure to explore a ternary mixture diagram to find the appropriate gradient profile in liquid chromatography with fluorescence detector. Application to determine four primary aromatic amines in napkins. Journal of Chromatography A, 2022, 1676, 463252.	1.8	1
3	Simultaneous class-modelling in chemometrics: A generalization of Partial Least Squares class modelling for more than two classes by using error correcting output code matrices. Chemometrics and Intelligent Laboratory Systems, 2022, 227, 104614.	1.8	6
4	Principal component regression that minimizes the sum of the squares of the relative errors: Application in multivariate calibration models. Journal of Chemometrics, 2021, 35, e3341.	0.7	0
5	A new approach based on inversion of a partial least squares model searching for a preset analytical target profile. Application to the determination of five bisphenols by liquid chromatography with diode array detector. Analytica Chimica Acta, 2021, 1149, 338217.	2.6	14
6	Partial least squares model inversion in the chromatographic determination of triazines in water. Microchemical Journal, 2021, 164, 105971.	2.3	6
7	Determination of polymer additive residues that migrate from coffee capsules by means of stir bar sorptive extraction-gas chromatography-mass spectrometry and PARAFAC decomposition. Food Packaging and Shelf Life, 2021, 28, 100664.	3.3	5
8	Handling Variables, via Inversion of Partial Least Squares Models for Class-Modelling, to Bring Defective Items to Non-Defective Ones. Frontiers in Chemistry, 2021, 9, 681958.	1.8	2
9	HPLC-DAD and PARAFAC for the determination of bisphenol-A and another four bisphenols migrating from BPA-free polycarbonate glasses. Microchemical Journal, 2021, 168, 106413.	2.3	11
10	Method operable design region obtained with a partial least squares model inversion in the determination of ten polycyclic aromatic hydrocarbons by liquid chromatography with fluorescence detection. Journal of Chromatography A, 2021, 1657, 462577.	1.8	11
11	A modified entropy-based performance criterion for class-modelling with multiple classes. Chemometrics and Intelligent Laboratory Systems, 2021, 217, 104423.	1.8	3
12	Unequivocal identification and quantification of PAHs content in ternary synthetic mixtures and in smoked tuna by means of excitation-emission fluorescence spectroscopy coupled with PARAFAC. Microchemical Journal, 2020, 154, 104561.	2.3	12
13	Quality of Analytical Measurements: Univariate Regression. , 2020, , 71-105.		3
14	Three-way PARAFAC decomposition of chromatographic data for the unequivocal identification and quantification of compounds in a regulatory framework. Chemometrics and Intelligent Laboratory Systems, 2020, 200, 104003.	1.8	18
15	Impact of the pretreatment of ATR-FTIR signals on the figures of merit when PLS is used. Chemometrics and Intelligent Laboratory Systems, 2020, 201, 104006.	1.8	8
16	Residual spaces in latent variables model inversion and their impact in the design space for given quality characteristics. Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104040.	1.8	8
17	Procedure to build a signal transfer set, independent of the target analytes, between a portable fluorimeter based on light-emitting diodes and a master fluorimeter. Analytica Chimica Acta, 2020, 1106, 33-41.	2.6	0
18	Quality of Analytical Measurements: Statistical Methods for InternalÂValidation. , 2020, , 1-52.		1

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19	Improvement in the identification and quantification of UV filters and additives in sunscreen cosmetic creams by gas chromatography/mass spectrometry through three-way calibration techniques. Talanta, 2019, 205, 120156.	2.9	16
20	Detection of cold chain breaks using partial least squares-class modelling based on biogenic amine profiles in tuna. Talanta, 2019, 202, 443-451.	2.9	3
21	Kinetic models of migration of melamine and formaldehyde from melamine kitchenware with data of liquid chromatography. Journal of Chromatography A, 2019, 1599, 115-124.	1.8	10
22	Fluorescence determination of cochineal in strawberry jam in the presence of carmoisine as a quencher by means of four-way PARAFAC decomposition. Food Chemistry, 2019, 290, 178-186.	4.2	13
23	Signal transfer with excitation-emission matrices between a portable fluorimeter based on light-emitting diodes and a master fluorimeter. Sensors and Actuators B: Chemical, 2019, 285, 240-247.	4.0	6
24	The behaviour of Tenax as food simulant in the migration of polymer additives from food contact materials by means of gas chromatography/mass spectrometry and PARAFAC. Journal of Chromatography A, 2019, 1589, 18-29.	1.8	23
25	Determination of cochineal and erythrosine in cherries in syrup in the presence of quenching effect by means of excitation-emission fluorescence data and three-way PARAFAC decomposition. Talanta, 2019, 196, 153-162.	2.9	13
26	D-Optimal Design and PARAFAC as Useful Tools for the Optimisation of Signals from Fluorescence Spectroscopy Prior to the Characterisation of Green Tea Samples. Food Analytical Methods, 2019, 12, 761-772.	1.3	3
27	Effect of the cleaning procedure of Tenax on its reuse in the determination of plasticizers after migration by gas chromatography/mass spectrometry. Talanta, 2018, 182, 505-522.	2.9	5
28	Easy-to-use procedure to optimise a chromatographic method. Application in the determination of bisphenol-A and phenol in toys by means of liquid chromatography with fluorescence detection. Journal of Chromatography A, 2018, 1534, 93-100.	1.8	20
29	Study of the effect of the presence of silver nanoparticles on migration of bisphenol A from polycarbonate glasses into food simulants. Chemometrics and Intelligent Laboratory Systems, 2018, 176, 66-73.	1.8	8
30	Impact of time and temperature of storage on the spoilage of swordfish and the evolution of biogenic amines through a multiway model. Journal of Chemometrics, 2018, 32, e2965.	0.7	2
31	A computational approach to partial least squares model inversion in the framework of the process analytical technology and quality by design initiatives. Chemometrics and Intelligent Laboratory Systems, 2018, 182, 70-78.	1.8	9
32	Combining excitation-emission matrix fluorescence spectroscopy, parallel factor analysis, cyclodextrin-modified micellar electrokinetic chromatography and partial least squares class-modelling for green tea characterization. Journal of Pharmaceutical and Biomedical Analysis, 2018, 159, 311-317.	1.4	15
33	Migration test of Bisphenol A from polycarbonate cups using excitation-emission fluorescence data with parallel factor analysis. Talanta, 2017, 167, 367-378.	2.9	42
34	Desirability functions as response in a <scp>d</scp>â€optimal design for evaluating the extraction and purification steps of six tranquillizers and an antiâ€adrenergic by liquid chromatographyâ€tandem mass spectrometry. Journal of Chemometrics, 2016, 30, 58-69.	0.7	4
35	A new multiresponse optimization approach in combination with a D-Optimal experimental design for the determination of biogenic amines in fish by HPLC-FLD. Analytica Chimica Acta, 2016, 945, 31-38.	2.6	30
36	A useful tool for computation and interpretation of trading-off solutions through pareto-optimal front in the field of experimental designs for mixtures. Chemometrics and Intelligent Laboratory Systems, 2016, 158, 210-217.	1.8	10

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37	Dealing with the ubiquity of phthalates in the laboratory when determining plasticizers by gas chromatography/mass spectrometry and PARAFAC. Journal of Chromatography A, 2016, 1464, 124-140.	1.8	15
38	Migration kinetics of primary aromatic amines from polyamide kitchenware: Easy and fast screening procedure using fluorescence. Talanta, 2016, 160, 46-55.	2.9	21
39	Distribution free methods to model the content of biogenic amines in Spanish wines. Chemometrics and Intelligent Laboratory Systems, 2016, 155, 191-199.	1.8	11
40	Robustness testing in the determination of seven drugs in animal muscle by liquid chromatography–tandem mass spectrometry. Chemometrics and Intelligent Laboratory Systems, 2016, 151, 172-180.	1.8	7
41	Design of bespoke lightweight cement mortars containing waste expanded polystyrene by experimental statistical methods. Materials and Design, 2016, 89, 901-912.	3.3	27
42	Parallel factor analysis for monitoring data from a grape harvest in Qualified Designation of Origin Rioja including spatial and temporal variability. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 347-353.	1.8	4
43	Usefulness of PARAFAC for the Quantification, Identification, and Description of Analytical Data. Data Handling in Science and Technology, 2015, , 37-81.	3.1	19
44	Standard addition method based on four-way PARAFAC decomposition to solve the matrix interferences in the determination of carbamate pesticides in lettuce using excitation–emission fluorescence data. Talanta, 2015, 138, 86-99.	2.9	25
45	Determination of dichlobenil and its major metabolite (BAM) in onions by PTV–GC–MS using PARAFAC2 and experimental design methodology. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 92-108.	1.8	18
46	Identification and quantification of carbamate pesticides in dried lime tree flowers by means of excitation-emission molecular fluorescence and parallel factor analysis when quenching effect exists. Analytica Chimica Acta, 2014, 820, 9-22.	2.6	27
47	Ad-hoc blocked design for the robustness study in the determination of dichlobenil and 2,6-dichlorobenzamide in onions by programmed temperature vaporization-gas chromatography–mass spectrometry. Journal of Chromatography A, 2014, 1370, 187-199.	1.8	3
48	Optimum pH for the determination of bisphenols and their corresponding diglycidyl ethers by gas chromatography–mass spectrometry. Migration kinetics of bisphenol A from polycarbonate glasses. Journal of Chromatography A, 2014, 1360, 23-38.	1.8	18
49	Optimization of a headspace solid-phase microextraction and gas chromatography/mass spectrometry procedure for the determination of aromatic amines in water and in polyamide spoons. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 121-135.	1.8	34
50	Selection of nearly orthogonal blocks in 'ad-hoc' experimental designs. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 109-120.	1.8	6
51	Modelling phenolic and technological maturities of grapes by means of the multivariate relation between organoleptic and physicochemical properties. Analytica Chimica Acta, 2013, 761, 53-61.	2.6	33
52	Optimization of a GC/MS procedure that uses parallel factor analysis for the determination of bisphenols and their diglycidyl ethers after migration from polycarbonate tableware. Talanta, 2013, 106, 266-280.	2.9	45
53	D-optimal experimental design coupled with parallel factor analysis 2 decomposition a useful tool in the determination of triazines in oranges by programmed temperature vaporization–gas chromatography–mass spectrometry when using dispersive-solid phase extraction. Journal of Chromatography A, 2013, 1288, 111-126.	1.8	16
54	Experimental design for the optimization of the derivatization reaction in determining chlorophenols and chloroanisoles by headspace-solid-phase microextraction–gas chromatography/mass spectrometry. Journal of Chromatography A, 2013, 1296, 179-195.	1.8	19

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55	On the construction of experimental designs for a given task by jointly optimizing several quality criteria: Pareto-optimal experimental designs. Analytica Chimica Acta, 2012, 754, 39-46.	2.6	11
56	Prediction of Zamorano cheese quality by near-infrared spectroscopy assessing false non-compliance and false compliance at minimum permitted limits stated by designation of origin regulations. Talanta, 2012, 99, 558-565.	2.9	18
57	Develop of a multiway chemometric-based analytical method fulfilling regulatory identification criteria: Application to GC–MS pesticide residue analysis. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012, 910, 122-137.	1.2	22
58	Optimization of headspace experimental factors to determine chlorophenols in water by means of headspace solid-phase microextraction and gas chromatography coupled with mass spectrometry and parallel factor analysis. Analytica Chimica Acta, 2012, 754, 20-30.	2.6	24
59	Advantages of a programmed temperature vaporizer inlet and parallel factor analysis in the determination of triazines in the presence of non-intentionally added substances by gas chromatography. Analytical and Bioanalytical Chemistry, 2012, 403, 1131-1143.	1.9	6
60	Usefulness of a PARAFAC decomposition in the fiber selection procedure to determine chlorophenols by means SPME-GC-MS. Analytical and Bioanalytical Chemistry, 2012, 403, 1095-1107.	1.9	11
61	D-optimal designs and N-way techniques to determine sulfathiazole in milk by molecular fluorescence spectroscopy. Analytica Chimica Acta, 2011, 707, 38-46.	2.6	17
62	Two class-modelling techniques that give families of class-models and their relation with the structure of the data. Analytical and Bioanalytical Chemistry, 2011, 399, 1941-1950.	1.9	0
63	Improving the visualization of the Pareto-optimal front for the multi-response optimization of chromatographic determinations. Analytica Chimica Acta, 2011, 687, 129-136.	2.6	22
64	Optimization of the derivatization reaction and the solid-phase microextraction conditions using a D-optimal design and three-way calibration in the determination of non-steroidal anti-inflammatory drugs in bovine milk by gas chromatography–mass spectrometry. Journal of Chromatography A, 2011, 1218, 4487-4497.	1.8	47
65	Optimization of a solid-phase extraction procedure in the fluorimetric determination of sulfonamides in milk using the second-order advantage of PARAFAC and D-optimal design. Analytical and Bioanalytical Chemistry, 2010, 396, 923-935.	1.9	11
66	A multivariate multianalyte screening method for sulfonamides in milk based on front-face fluorescence spectroscopy. Analytica Chimica Acta, 2010, 657, 136-146.	2.6	24
67	Tutorial on evaluation of type I and type II errors in chemical analyses: From the analytical detection to authentication of products and process control. Analytica Chimica Acta, 2010, 674, 123-142.	2.6	61
68	Class-modelling techniques that optimize the probabilities of false noncompliance and false compliance. Chemometrics and Intelligent Laboratory Systems, 2010, 103, 25-42.	1.8	12
69	Analysis of protein chromatographic profiles joint to partial least squares to detect adulterations in milk mixtures and cheeses. Talanta, 2010, 81, 255-264.	2.9	47
70	D-optimal design used to optimize a multi-response class-modelling method. Chemometrics and Intelligent Laboratory Systems, 2009, 95, 138-143.	1.8	8
71	Determination and identification, according to European Union Decision 2002/657/EC, of malachite green and its metabolite in fish by liquid chromatography–tandem mass spectrometry using an optimized extraction procedure and three-way calibration. Journal of Chromatography A, 2009, 1216, 5472-5482.	1.8	45
72	Usefulness of parallel factor analysis to handle the matrix effect in the fluorescence determination of tetracycline in whey milk. Analytica Chimica Acta, 2009, 632, 42-51.	2.6	32

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73	Identification and quantification of ciprofloxacin in urine through excitation-emission fluorescence and three-way PARAFAC calibration. Analytica Chimica Acta, 2009, 642, 193-205.	2.6	31
74	Study of robustness based on n-way models in the spectrofluorimetric determination of tetracyclines in milk when quenching exists. Analytica Chimica Acta, 2009, 651, 149-158.	2.6	19
75	Fluorescence quantification of tetracycline in the presence of quenching matrix effect by means of a four-way model. Talanta, 2009, 77, 1129-1136.	2.9	33
76	Response Surface Methodology. , 2009, , 345-390.		86
77	Quality of Analytical Measurements: Statistical Methods for Internal Validation. , 2009, , 17-76.		2
78	Quality of Analytical Measurements: Univariate Regression. , 2009, , 127-169.		9
79	Potential of front face fluorescence associated to PLS regression to predict nutritional parameters in heat treated infant formula models. Analytica Chimica Acta, 2008, 606, 151-158.	2.6	30
80	Pareto-optimal front as a tool to study the behaviour of experimental factors in multi-response analytical procedures. Analytica Chimica Acta, 2008, 624, 210-222.	2.6	23
81	How to search the experimental conditions that improve a Partial Least Squares calibration model. Chemometrics and Intelligent Laboratory Systems, 2008, 92, 71-82.	1.8	10
82	Advantages of PARAFAC calibration in the determination of malachite green and its metabolite in fish by liquid chromatography–tandem mass spectrometry. Journal of Chromatography A, 2008, 1187, 1-10.	1.8	43
83	Optimization of a FIA system with amperometric detection by means of a desirability functionDetermination of sulfadiazine, sulfamethazine and sulfamerazine in milk. Talanta, 2008, 75, 274-283.	2.9	19
84	Chapter 1 Introduction to Ranking Methods. Data Handling in Science and Technology, 2008, , 1-50.	3.1	3
85	Analysis of interferents by means a D-optimal screening design and calibration using partial least squares regression in the spectrophotometric determination of Cr(VI). Talanta, 2007, 71, 1599-1609.	2.9	15
86	Performance characteristics according to Commission Decision 2002/657/EC in the fluorimetric determination of tetracycline in the absence and in the presence of magnesium. Luminescence, 2007, 22, 518-526.	1.5	4
87	Quantitative determination in chromatographic analysis based on n-way calibration strategies. Journal of Chromatography A, 2007, 1158, 94-110.	1.8	85
88	Multiresponse optimization and parallel factor analysis, useful tools in the determination of estrogens by gas chromatography–mass spectrometry. Journal of Chromatography A, 2007, 1157, 358-368.	1.8	40
89	Rapid determination of sulfonamides in milk samples using fluorescence spectroscopy and class modeling with n-way partial least squares. Analytica Chimica Acta, 2007, 585, 350-360.	2.6	31
90	Validation of an analytical method to determine sulfamides in kidney by HPLC-DAD and PARAFAC2 with first-order derivative chromatograms. Analytica Chimica Acta, 2007, 587, 222-234.	2.6	42

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91	Focused microwave-assisted Soxhlet extraction of acorn oil for determination of the fatty acid profile by GC–MS. Comparison with conventional and standard methods. Analytical and Bioanalytical Chemistry, 2007, 388, 451-462.	1.9	28
92	Optimization of analytical conditions and validation of a fluorescence method for the determination of sulfadiazine in milk. Analytical and Bioanalytical Chemistry, 2007, 388, 957-968.	1.9	5
93	Teaching chemometrics. Analytical and Bioanalytical Chemistry, 2007, 388, 1557-1560.	1.9	0
94	Robust regression techniquesA useful alternative for the detection of outlier data in chemical analysis. Talanta, 2006, 70, 499-512.	2.9	60
95	Sensitivity and specificity of PLS-class modelling for five sensory characteristics of dry-cured ham using visible and near infrared spectroscopy. Analytica Chimica Acta, 2006, 558, 125-131.	2.6	110
96	Capability of detection and three-way data. Analytica Chimica Acta, 2006, 559, 124-136.	2.6	43
97	Vectorial optimization as a methodogical alternative to desirability function. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 157-168.	1.8	31
98	The maintenance of a PARAFAC calibration and the second-order property: application to the determination of ciprofloxacin in presence of enrofloxacin by excitation–emission fluorescence. Analytica Chimica Acta, 2005, 544, 327-336.	2.6	22
99	Outliers in partial least squares regression. Analytica Chimica Acta, 2005, 544, 60-70.	2.6	28
100	Optimization of the chromatographic conditions for the determination of hormones by gas chromatography with mass spectrometry detection. Analytica Chimica Acta, 2005, 544, 26-35.	2.6	19
101	Usefulness of D-optimal designs and multicriteria optimization in laborious analytical procedures. Journal of Chromatography A, 2005, 1085, 190-198.	1.8	36
102	Methodology of multicriteria optimization in chemical analysis Some applications in stripping voltammetry. Talanta, 2005, 65, 246-254.	2.9	24
103	Maintenance of Soft Calibration Models in the Determination of Zinc, Cadmium, Lead and Copper by Differential Pulse Anodic Stripping Voltammetry. Electroanalysis, 2004, 16, 748-756.	1.5	10
104	Selecting variables for k-means cluster analysis by using a genetic algorithm that optimises the silhouettes. Analytica Chimica Acta, 2004, 515, 87-100.	2.6	162
105	Minimum value assured by a method to determine gold in alloys by using laser-induced breakdown spectroscopy and partial least-squares calibration model. Analytica Chimica Acta, 2004, 515, 151-157.	2.6	26
106	Building robust calibration models for the analysis of estrogens by gas chromatography with mass spectrometry detection. Analytica Chimica Acta, 2004, 526, 139-146.	2.6	33
107	Determination of quinolones by fluorescent excitation emission. Talanta, 2004, 64, 442-451.	2.9	12
108	Advances in methodology for the validation of methods according to the International Organization for Standardization. Journal of Chromatography A, 2003, 992, 11-27.	1.8	72

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109	Optimisation of a flow injection system with electrochemical detection using the desirability function. Analytica Chimica Acta, 2003, 479, 173-184.	2.6	76
110	Multivariate analytical sensitivity in the determination of selenium, copper, lead and cadmium by stripping voltammetry when using soft calibration. Analytica Chimica Acta, 2003, 489, 85-94.	2.6	19
111	Partial least squares fine-tuning by a bootstrap estimated signalâ€"noise relation to weight the loadings. Chemometrics and Intelligent Laboratory Systems, 2003, 68, 83-96.	1.8	0
112	Capability of detection of an analytical method evaluating false positive and false negative (ISO 11843) with partial least squares. Chemometrics and Intelligent Laboratory Systems, 2003, 69, 21-33.	1.8	106
113	A study of robustness with multivariate calibration. Application to the polarographic determination of benzaldehyde. Talanta, 2002, 56, 1039-1048.	2.9	29
114	Determination of the capability of detection of a hyphenated method: application to spectroelectrochemistry. Chemometrics and Intelligent Laboratory Systems, 2002, 61, 63-74.	1.8	25
115	Preliminary results of an interlaboratory study of chemometric software and methods on NIR data. Predicting the content of crude protein and water in forages. Chemometrics and Intelligent Laboratory Systems, 2002, 63, 93-105.	1.8	16
116	Analysis and comparison of SIMCA models for denominations of origin of wines from de Canary Islands (Spain) builds by means of their trace and ultratrace metals content. Analytica Chimica Acta, 2002, 472, 161-174.	2.6	35
117	Soft calibration in a flow system with electrochemical detection. Analytica Chimica Acta, 2001, 446, 267-277.	2.6	13
118	Capability of discrimination: application to soft calibration methods. Analytica Chimica Acta, 2001, 446, 295-309.	2.6	15
119	Psychophysical parameters of colour and the chemometric characterisation of wines of the certified denomination of origin â€˜Riojaâ€™. Analytica Chimica Acta, 2001, 446, 157-167.	2.6	15
120	Quality control decisions with near infrared data. Chemometrics and Intelligent Laboratory Systems, 2000, 53, 69-80.	1.8	25
121	Handling intrinsic non-linearity in near-infrared reflectance spectroscopy. Chemometrics and Intelligent Laboratory Systems, 1999, 49, 215-224.	1.8	45
122	Performance of the orthogonal least median sqares regression. Analytica Chimica Acta, 1997, 348, 11-18.	2.6	2
123	Multivariate calibration transfer applied to the routine polarographic determination of copper, lead, cadmium and zinc. Analytica Chimica Acta, 1997, 348, 51-59.	2.6	47
124	Using continuum regression for quantitative analysis with overlapping signals obtained by differential pulse polarography. Chemometrics and Intelligent Laboratory Systems, 1996, 34, 245-262.	1.8	28
125	DETARCHI: A program for detection limits with specified assurance probabilities and characteristic curves of detection. TrAC - Trends in Analytical Chemistry, 1994, 13, 1-6.	5.8	124
126	A program for non-orthogonal rotation in factor analysis. TrAC - Trends in Analytical Chemistry, 1993, 12, 226-230.	5.8	5