MarÃa Cruz Ortiz

List of Publications by Year
in descending order

126	2,980	172207	223531
papers	citations	29	46
		h-index	g-index

126	126	126	2603
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	Response Surface Methodology. , 2009, , 345-390.		86
6	Quantitative determination in chromatographic analysis based on n-way calibration strategies. Journal of Chromatography A, 2007, 1158, 94-110.	1.8	85
7	Optimisation of a flow injection system with electrochemical detection using the desirability function. Analytica Chimica Acta, 2003, 479, 173-184.	2.6	76
8	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
9	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
10	Robust regression techniquesA useful alternative for the detection of outlier data in chemical analysis. Talanta, 2006, 70, 499-512.	2.9	60
11	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
12	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
13	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
14	Handling intrinsic non-linearity in near-infrared reflectance spectroscopy. Chemometrics and Intelligent Laboratory Systems, 1999, 49, 215-224.	1.8	45
15	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
16	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
17	Capability of detection and three-way data. Analytica Chimica Acta, 2006, 559, 124-136.	2.6	43
18	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

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19	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
20	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
21	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
22	Usefulness of D-optimal designs and multicriteria optimization in laborious analytical procedures. Journal of Chromatography A, 2005, 1085, 190-198.	1.8	36
23	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
24	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
25	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
26	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
27	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
28	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
29	Vectorial optimization as a methodogical alternative to desirability function. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 157-168.	1.8	31
30	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
31	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
32	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
33	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
34	A study of robustness with multivariate calibration. Application to the polarographic determination of benzaldehyde. Talanta, 2002, 56, 1039-1048.	2.9	29
35	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
36	Outliers in partial least squares regression. Analytica Chimica Acta, 2005, 544, 60-70.	2.6	28

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37	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
38	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
39	Design of bespoke lightweight cement mortars containing waste expanded polystyrene by experimental statistical methods. Materials and Design, 2016, 89, 901-912.	3.3	27
40	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
41	Quality control decisions with near infrared data. Chemometrics and Intelligent Laboratory Systems, 2000, 53, 69-80.	1.8	25
42	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
43	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
44	Methodology of multicriteria optimization in chemical analysis Some applications in stripping voltammetry. Talanta, 2005, 65, 246-254.	2.9	24
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	Migration kinetics of primary aromatic amines from polyamide kitchenware: Easy and fast screening procedure using fluorescence. Talanta, 2016, 160, 46-55.	2.9	21
53	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
54	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

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55	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
56	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
57	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
58	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
59	Usefulness of PARAFAC for the Quantification, Identification, and Description of Analytical Data. Data Handling in Science and Technology, 2015, , 37-81.	3.1	19
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	Capability of discrimination: application to soft calibration methods. Analytica Chimica Acta, 2001, 446, 295-309.	2.6	15
69	Psychophysical parameters of colour and the chemometric characterisation of wines of the certified denomination of origin 'Rioja'. Analytica Chimica Acta, 2001, 446, 157-167.	2.6	15
70	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
71	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
72	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

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73	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
74	Soft calibration in a flow system with electrochemical detection. Analytica Chimica Acta, 2001, 446, 267-277.	2.6	13
75	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
76	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
77	Determination of quinolones by fluorescent excitation emission. Talanta, 2004, 64, 442-451.	2.9	12
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	Quality of Analytical Measurements: Univariate Regression. , 2009, , 127-169.		9

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91	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
92	D-optimal design used to optimize a multi-response class-modelling method. Chemometrics and Intelligent Laboratory Systems, 2009, 95, 138-143.	1.8	8
93	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
94	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
95	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
96	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
97	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
98	Selection of nearly orthogonal blocks in 'ad-hoc' experimental designs. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 109-120.	1.8	6
99	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
100	Partial least squares model inversion in the chromatographic determination of triazines in water. Microchemical Journal, 2021, 164, 105971.	2.3	6
101	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
102	A program for non-orthogonal rotation in factor analysis. TrAC - Trends in Analytical Chemistry, 1993, 12, 226-230.	5.8	5
103	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
104	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
105	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
106	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
107	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
108	Desirability functions as response in a d‐optimal design for evaluating the extraction and purification steps of six tranquillizers and an anti‐adrenergic by liquid chromatography–tandem mass spectrometry. Journal of Chemometrics, 2016, 30, 58-69.	0.7	4

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109	Chapter 1 Introduction to Ranking Methods. Data Handling in Science and Technology, 2008, , 1-50.	3.1	3
110	Ad-hoc blocked design for the robustness study in the determination of dichlobenil and 2,6-dichlorobenzamide in onions by programmed temperature vaporization-gas chromatographyâ€"mass spectrometry. Journal of Chromatography A, 2014, 1370, 187-199.	1.8	3
111	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
112	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
113	Quality of Analytical Measurements: Univariate Regression. , 2020, , 71-105.		3
114	A modified entropy-based performance criterion for class-modelling with multiple classes. Chemometrics and Intelligent Laboratory Systems, 2021, 217, 104423.	1.8	3
115	Performance of the orthogonal least median sqares regression. Analytica Chimica Acta, 1997, 348, 11-18.	2.6	2
116	Quality of Analytical Measurements: Statistical Methods for Internal Validation. , 2009, , 17-76.		2
117	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
118	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
119	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
120	Quality of Analytical Measurements: Statistical Methods for InternalÂValidation. , 2020, , 1-52.		1
121	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
122	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
123	Teaching chemometrics. Analytical and Bioanalytical Chemistry, 2007, 388, 1557-1560.	1.9	0
124	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
125	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
126	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