## Santiago Maspoch

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Near-infrared spectroscopy in the pharmaceutical industry. Analyst, The, 1998, 123, 135R-150R.	1.7	212
2	NIR calibration in non-linear systems: different PLS approaches and artificial neural networks. Chemometrics and Intelligent Laboratory Systems, 2000, 50, 75-82.	1.8	148
3	Study of pharmaceutical samples by NIR chemical-image and multivariate analysis. TrAC - Trends in Analytical Chemistry, 2008, 27, 696-713.	5.8	139
4	Solving GC-MS problems with PARAFAC2. TrAC - Trends in Analytical Chemistry, 2008, 27, 714-725.	5.8	134
5	Simultaneous kinetic-spectrophotometric determination of levodopa and benserazide by bi- and three-way partial least squares calibration. Talanta, 2000, 53, 627-637.	2.9	95
6	Diode-array detectors in flow-injection analysis Mixture resolution by multi-wavelength analysis. Talanta, 1987, 34, 987-993.	2.9	94
7	Near Infrared Spectrometry and Pattern Recognition as Screening Methods for the Authentication of Virgin Olive Oils of Very Close Geographical Origins. Journal of Near Infrared Spectroscopy, 2000, 8, 45-52.	0.8	74
8	Effect of Data Preprocessing Methods in Near-Infrared Diffuse Reflectance Spectroscopy for the Determination of the Active Compound in a Pharmaceutical Preparation. Applied Spectroscopy, 1997, 51, 240-246.	1.2	73
9	Artificial Neural Networks for Multicomponent Kinetic Determinations. Analytical Chemistry, 1995, 67, 4477-4483.	3.2	71
10	Calibration in non-linear near infrared reflectance spectroscopy: a comparison of several methods. Analytica Chimica Acta, 1999, 384, 207-214.	2.6	70
11	An effective microfluidic based liquid-phase microextraction device (μLPME) for extraction of non-steroidal anti-inflammatory drugs from biological and environmental samples. Analytica Chimica Acta, 2016, 946, 56-63.	2.6	65
12	Quantitation of the active compound and major excipients in a pharmaceutical formulation by near infrared diffuse reflectance spectroscopy with fibre optical probe. Analytica Chimica Acta, 1996, 333, 147-156.	2.6	62
13	Determination of olive oil free fatty acid by fourier transform infrared spectroscopy. JAOCS, Journal of the American Oil Chemists' Society, 1999, 76, 611-616.	0.8	62
14	Separation of profen enantiomers by capillary electrophoresis using cyclodextrins as chiral selectors. Journal of Chromatography A, 1998, 793, 165-175.	1.8	61
15	Analytical control of pharmaceutical production steps by near infrared reflectance spectroscopy. Analytica Chimica Acta, 1999, 392, 237-246.	2.6	61
16	Enhanced chromatographic fingerprinting of herb materials by multi-wavelength selection and chemometrics. Analytica Chimica Acta, 2012, 710, 40-49.	2.6	59
17	A mixed hard- and soft-modelling approach to study and monitor enzymatic systems in biological fluids. Analytica Chimica Acta, 2006, 567, 245-254.	2.6	55
18	Multi-wavelength high-performance liquid chromatographic fingerprints and chemometrics to predict the antioxidant activity of Turnera diffusa as part of its quality control. Journal of Chromatography A, 2012, 1235, 68-76.	1.8	50

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19	A mixed hard- and soft-modelling approach for the quantitative determination of oxipurines and uric acid in human urine. Analytica Chimica Acta, 2006, 567, 236-244.	2.6	49
20	Fast assessment of the surface distribution of API and excipients in tablets using NIR-hyperspectral imaging. International Journal of Pharmaceutics, 2011, 411, 27-35.	2.6	49
21	Determination of sulphur dioxide by flow injection analysis with amperometric detection. Analytica Chimica Acta, 1986, 179, 445-451.	2.6	45
22	Handling intrinsic non-linearity in near-infrared reflectance spectroscopy. Chemometrics and Intelligent Laboratory Systems, 1999, 49, 215-224.	1.8	45
23	Application of a photodiode array detector to multi-component determination by flow injection analysis. Analyst, The, 1987, 112, 619-622.	1.7	44
24	Kinetic spectrophotometric determination of Ga(III)-Al(III) mixtures by stopped-flow injection analysis using principal component regression. Talanta, 1993, 40, 261-267.	2.9	43
25	Principal Component Regression for Mixture Resolution in Control Analysis by UV-Visible Spectrophotometry. Applied Spectroscopy, 1994, 48, 37-43.	1.2	43
26	Artificial neural networks and partial least squares regression for pseudo-first-order with respect to the reagent multicomponent kinetic-spectrophotometric determinations. Analyst, The, 1996, 121, 395-400.	1.7	41
27	The influence of particle size on the intensity and reproducibility of Raman spectra of compacted samples. Vibrational Spectroscopy, 2019, 100, 48-56.	1.2	40
28	Simultaneous multiwavelength spectrophotometric quantitation of active components in analgesic formulations. Comparative study of three calculation methods. Journal of Pharmaceutical and Biomedical Analysis, 1988, 6, 765-772.	1.4	39
29	Control analysis of a pharmaceutical preparation by near-infrared reflectance spectroscopy. Analytica Chimica Acta, 1994, 298, 183-191.	2.6	38
30	Development and validation of a method for the analysis of a pharmaceutical preparation by nearâ€infrared diffuse reflectance spectroscopy. Journal of Pharmaceutical Sciences, 1999, 88, 551-556.	1.6	38
31	Determination of polymorphic purity by near infrared spectrometry. Analytica Chimica Acta, 2000, 407, 247-254.	2.6	38
32	Influence of the procedure used to prepare the calibration sample set on the performance of near infrared spectroscopy in quantitative pharmaceutical analyses. Analyst, The, 2001, 126, 1129-1134.	1.7	38
33	A simple and fast Double-Flow microfluidic device based liquid-phase microextraction (DF-µLPME) for the determination of parabens in water samples. Talanta, 2017, 165, 496-501.	2.9	37
34	Kinetic spectrophotometric method for analyzing mixtures of metal ions by stopped-flow injection analysis using partial least-squares regression. Analytical Chemistry, 1994, 66, 2905-2911.	3.2	36
35	Strategies for Constructing the Calibration Set in the Determination of Active Principles in Pharmaceuticals by Near Infrared Diffuse Reflectance Spectrometry. Analyst, The, 1997, 122, 761-765.	1.7	36
36	Three-way partial least-squares regression for the simultaneous kinetic-enzymatic determination of xanthine and hypoxanthine in human urine. Analytical and Bioanalytical Chemistry, 2005, 382, 1380-1388.	1.9	36

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37	Simultaneous kinetic spectrophotometric determination of o-, m-and p-aminophenol using partial least squares calibration. Analyst, The, 1996, 121, 407-412.	1.7	35
38	Determination of Finishing Oils in Acrylic Fibres by Near-infrared Reflectance Spectrometry. Analyst, The, 1997, 122, 777-781.	1.7	33
39	Near-infrared analytical control of pharmaceuticals. A single calibration model from mixed phase to coated tablets. Analyst, The, 1998, 123, 2307-2312.	1.7	33
40	Spectrophotometric determination of pharmaceutical dosages by partial least-squares calibration. Journal of Pharmaceutical and Biomedical Analysis, 1994, 12, 509-514.	1.4	31
41	Partial least-squares regression for multicomponent kinetic determinations in linear and non-linear systems. Analytica Chimica Acta, 1995, 303, 309-320.	2.6	31
42	Effect of orthogonal signal correction on the determination of compounds with very similar near infrared spectra. Analytica Chimica Acta, 2001, 431, 303-311.	2.6	30
43	Application of near infrared spectral fingerprinting and pattern recognition techniques for fast identification of Eleutherococcus senticosus. Food Research International, 2011, 44, 557-565.	2.9	30
44	Spectrophotometric Analysis of a Pharmaceutical Preparation by Principal Component Regression. Journal of Pharmaceutical Sciences, 1993, 82, 834-837.	1.6	29
45	Kinetic spectrophotometric determination of hydrocortisone acetate in a pharmaceutical preparation by use of partial least- squares regression. Analyst, The, 1999, 124, 911-915.	1.7	29
46	Evaluation of classical and three-way multivariate calibration procedures in kinetic-spectrophotometric analysis. Analytica Chimica Acta, 2000, 424, 115-126.	2.6	29
47	Geographical Origin Classification of Petroleum Crudes from Near-Infrared Spectra of Bitumens. Applied Spectroscopy, 2001, 55, 834-839.	1.2	29
48	Determination of ascorbic acid in pharmaceutical preparations by near infrared reflectance spectroscopy. Talanta, 1993, 40, 1671-1676.	2.9	28
49	UV-spectrophotometric determination of ketoprofen and paraben in a gel preparation by partial least-squares calibration. Fresenius' Journal of Analytical Chemistry, 1997, 357, 967-972.	1.5	28
50	Simultaneous enzymatic spectrophotometric determination of ethanol and methanol by use of artificial neural networks for calibration. Analytica Chimica Acta, 1999, 398, 83-92.	2.6	28
51	Parallel factor analysis combined with PLS regression applied to the on-line monitoring of Pichia pastoris cultures. Analytical and Bioanalytical Chemistry, 2006, 385, 1281-1288.	1.9	28
52	Raman spectroscopy as a complementary tool to assess the content uniformity of dosage units in break-scored warfarin tablets. International Journal of Pharmaceutics, 2014, 465, 299-305.	2.6	28
53	Chiral and nonchiral determination of ketoprofen in pharmaceuticals by capillary zone electrophoresis. Journal of Chromatography A, 1998, 799, 301-307.	1.8	27
54	Enzymatic synthesis of a thiolated chitosan-based wound dressing crosslinked with chicoric acid. Journal of Materials Chemistry B, 2018, 6, 7943-7953.	2.9	27

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55	Use of diode-array detectors for the simultaneous spectrophotometric determination of calcium and magnesium by flow injection. Analytica Chimica Acta, 1989, 224, 23-30.	2.6	26
56	A simple method for spectrophotometric determination of two-components with overlapped spectra. Journal of Chemical Education, 1989, 66, 178.	1.1	26
57	Determination of water in ferrous lactate by near infrared reflectance spectroscopy with a fibre-optic probe. Journal of Pharmaceutical and Biomedical Analysis, 1997, 16, 255-262.	1.4	26
58	Development and validation of a near infrared method for the analytical control of a pharmaceutical preparation in three steps of the manufacturing process. Fresenius' Journal of Analytical Chemistry, 2000, 368, 534-539.	1.5	26
59	On-line parallel factor analysis. A step forward in the monitoring of bioprocesses in real time. Chemometrics and Intelligent Laboratory Systems, 2008, 92, 44-52.	1.8	26
60	Determination of water in lubricating oils by mid- and near-infrared spectroscopy. Mikrochimica Acta, 1998, 128, 235-239.	2.5	25
61	Circular dichroism spectra of cyclodextrins–ketoprofen inclusion complexes. Analytica Chimica Acta, 2000, 407, 233-245.	2.6	24
62	Application of partial least-squares regression to the resolution of highly correlated spectra. Simultaneous spectrofluorimetric determination of Al, Ga and In. Talanta, 1996, 43, 1489-1496.	2.9	23
63	Wavelength Calibration Transfer between Diode Array UV-Visible Spectrophotometers. Applied Spectroscopy, 1995, 49, 593-597.	1.2	21
64	Use of near-infrared spectrometry in control analyses of acrylic fibre manufacturing processes. Analytica Chimica Acta, 1999, 383, 291-298.	2.6	21
65	Development and validation of methods for the determination of miokamycin in various pharmaceutical preparations by use of near infrared reflectance spectroscopy. Analyst, The, 1999, 124, 1089-1092.	1.7	21
66	An Introduction to Multivariate Curve Resolution-Alternating Least Squares: Spectrophotometric Study of the Acid–Base Equilibria of 8-Hydroxyquinoline-5-sulfonic Acid. Journal of Chemical Education, 2007, 84, 1190.	1.1	21
67	Implementation of enhanced correlation maps in near infrared chemical images: Application in pharmaceutical research. Talanta, 2009, 79, 657-664.	2.9	21
68	Multi-component analysis of concentrated solutions by flow-injection analysis with zone sampling and partial least-squares resolution. Analytica Chimica Acta, 1992, 259, 219-224.	2.6	20
69	Simultaneous determination of metal ions. Analytica Chimica Acta, 1989, 226, 271-279.	2.6	19
70	Analysis of cotton–polyester yarns by near-infrared reflectance spectroscopy. Analyst, The, 1994, 119, 1779-1785.	1.7	19
71	Determination of physico-chemical parameters for bitumens using near infrared spectroscopy. Analytica Chimica Acta, 2001, 434, 133-141.	2.6	19
72	Impedance model for voltage optimization of parabens extraction in an electromembrane millifluidic device. Journal of Chromatography A, 2020, 1625, 461270.	1.8	18

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73	Simultaneous determination of metal ions. Analytica Chimica Acta, 1989, 222, 271-279.	2.6	17
74	On-line monitoring of starch enzymatic hydrolysis by near- infrared spectroscopy. Analyst, The, 2000, 125, 749-752.	1.7	17
75	An efficient microfluidic device based on electromembrane extraction for the simultaneous extraction of acidic and basic drugs. Analytica Chimica Acta, 2021, 1160, 338448.	2.6	17
76	Catalytic determination of manganese at ultra-trace levels by flow injection analysis. Analyst, The, 1986, 111, 69-72.	1.7	16
77	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
78	Direct determination of leather dyes by visible reflectance spectroscopy using partial least-squares regression. Analytica Chimica Acta, 2000, 419, 209-214.	2.6	15
79	Determination of the penetration value of bitumens by near infrared spectroscopy. Analyst, The, 2000, 125, 1823-1828.	1.7	15
80	Determination of cyanide by a highly sensitive indirect spectrophotometric method. Talanta, 1984, 31, 85-87.	2.9	14
81	Simultaneous determination of two components by spectrofluorimetric techniques. Analytica Chimica Acta, 1990, 233, 159-163.	2.6	14
82	Partial least-squares regression for the quantitation of pharmaceutical dosages in control analyses. Journal of Pharmaceutical and Biomedical Analysis, 1996, 15, 329-338.	1.4	14
83	Simultaneous Spectrophotometric Determination of Levodopa and Benserazide in a Pharmaceutical. Analytical Letters, 2000, 33, 2701-2718.	1.0	14
84	5-phenylazo-8-aminoquinoline as a sensitive reagent for the extraction-spectrophotometric determination of palladium(II). Mikrochimica Acta, 1983, 81, 11-20.	2.5	13
85	Determination of physical properties of bitumens by use of near-infrared spectroscopy with neural networks. Joint modelling of linear and non-linear parameters. Analyst, The, 2001, 126, 378-382.	1.7	12
86	Evaluation of NIR and Raman spectroscopies for the quality analytical control of a solid pharmaceutical formulation with three active ingredients Microchemical Journal, 2020, 154, 104576.	2.3	12
87	Simultaneous Determination of Rubber Additives by FT-IR Spectrophotometry with Multivariate Calibration. Applied Spectroscopy, 1995, 49, 747-753.	1.2	11
88	Use of circular dichroism and artificial neural networks for the kinetic-spectrophotometric resolution of enantiomers. Analytica Chimica Acta, 2001, 431, 115-123.	2.6	11
89	Enhancing sensitivity and precision on NIR reflectance determination of an API at low concentration: Application to an hormonal preparation. Journal of Pharmaceutical and Biomedical Analysis, 2012, 60, 59-64.	1.4	11
90	Evaluation of a handheld near-infrared spectrophotometer for quantitative determination of two APIs in a solid pharmaceutical preparation. Analytical Methods, 2019, 11, 327-335.	1.3	11

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91	Flow Injection Amperometric Determination of Pharmaceuticals. Archiv Der Pharmazie, 1988, 321, 725-728.	2.1	10
92	Precision of a diode-array spectrophotometer. Analytica Chimica Acta, 1990, 234, 395-401.	2.6	10
93	Raman spectroscopy for the analytical quality control of low-dose break-scored tablets. Journal of Pharmaceutical and Biomedical Analysis, 2016, 124, 207-215.	1.4	9
94	Analysis of Multicomponent Spectra by the Simplex Method. Analytical Letters, 1992, 25, 543-560.	1.0	8
95	Simultaneous spectrophotometric determination of fat-soluble vitamins in multivitamin pharmaceutical preparations. Fresenius' Journal of Analytical Chemistry, 1995, 351, 315-319.	1.5	8
96	Expeditious identification and semi-quantification of Panax ginseng using near infrared spectral fingerprints and multivariate analysis. Analytical Methods, 2013, 5, 857.	1.3	8
97	Finding a reliable limit of detection in the NIR determination of residual moisture in a freeze-dried drug product. Journal of Pharmaceutical and Biomedical Analysis, 2020, 183, 113163.	1.4	8
98	Calibration in near Infrared Diffuse Reflectance Spectroscopy. A Comparative Study of Various Methods. Journal of Near Infrared Spectroscopy, 1997, 5, 67-75.	0.8	7
99	Determination of accelerators and antioxidants in vulcanized rubber by fourier transform infrared spectrophotometry. Analytica Chimica Acta, 1997, 353, 351-358.	2.6	7
100	Metal binding properties of three Cys2X2 (X = His, Asp) metallothionein-related peptides. Inorganica Chimica Acta, 1998, 278, 10-14.	1.2	7
101	Analytical control of a pharmaceutical formulation of sodium picosulfate by capillary zone electrophoresis. Biomedical Applications, 2001, 751, 29-36.	1.7	7
102	Diode array detectors in flow injection analysis. Simultaneous determination of rare earth metals with Arsenazo III. Fresenius' Journal of Analytical Chemistry, 1990, 338, 831-835.	1.5	6
103	Application of multicomponent spectrophotometry to analytical control of electroplating solutions. Fresenius' Journal of Analytical Chemistry, 1991, 340, 410-414.	1.5	6
104	Analytical control of organic additives in electrolytic baths by UV spectroscopy in combination with multivariate analysis. Fresenius' Journal of Analytical Chemistry, 1999, 363, 364-368.	1.5	6
105	Kinetic-spectrophotometric determination of theophylline, dyphylline, and proxyphylline by use of partial least-squares regression. Analytical and Bioanalytical Chemistry, 2002, 374, 33-38.	1.9	6
106	NIR reflectance determination of warfarin in a solid preparation commercialized at different API mass proportions. Analytical Methods, 2013, 5, 3858.	1.3	6
107	Simultaneous determination of metal ions. Catalytic oxidation of cobalt by metal ions when extracted with quinolin-8-ol. Analytica Chimica Acta, 1990, 230, 221-224.	2.6	5
108	Effect of Day-To-Day Noise on UV-Visible Spectrophotometric Control Analyses of Mixtures by Principal Component Regression. Applied Spectroscopy, 1996, 50, 576-582.	1.2	5

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109	Application of the Davidon-Fletcher-Powell algorithm to the resolution of multicomponent mixtures using UV-vis spectrophotometry. Analytica Chimica Acta, 1996, 327, 145-152.	2.6	5
110	Modelling of an environmental parameter by use of the alternating conditional expectation method. Chemometrics and Intelligent Laboratory Systems, 1999, 46, 31-39.	1.8	5
111	Use of Inverse Multiple Linear Regression (ILS) for the Analytical Control of Pharmaceutical Preparations. UV-Visible Spectrophotometric Quantitation of an Active Principal in the Presence of Absorbing Excipients. Analytical Letters, 1999, 32, 1169-1181.	1.0	5
112	Application of Representative Layer Theory to Near-Infrared Reflectance Spectra of Powdered Samples. Applied Spectroscopy, 2008, 62, 1363-1369.	1.2	5
113	Recent advances in sample pre-treatment for emerging methods in proteomic analysis. Talanta, 2017, 174, 738-751.	2.9	5
114	Fia Fluorimetric Determination of Calcium Pantothenate. Validation and Quantitation in Multivitamin Preparations. Analytical Letters, 1995, 28, 821-833.	1.0	4
115	8-Aminoquinoline and 5,7-Dihalogen Derivatives. Determination of Protonation Constants and Some Gravimetric Applications. Mikrochimica Acta, 1983, 81, 95-104.	2.5	3
116	Simultaneous spectrophotometric determination of Zinc(II) and Nickel(II) with 1-(2-pyridylazo)-2-naphthol. Mikrochimica Acta, 1992, 108, 53-59.	2.5	3
117	Spectrofluorimetric Identification of Polycyclic Aromatic Hydrocarbons at PPB Level. Analytical Letters, 1996, 29, 1603-1617.	1.0	3
118	Resolution of isomers of sorbitolparaben esters by chromatographic and electrophoretic techniques. Biomedical Applications, 2001, 752, 99-105.	1.7	3
119	Determination of carbohydrazide at trace and subtrace levels. Talanta, 1992, 39, 1313-1316.	2.9	2
120	Multi-component kinetic–spectrophotometric analysis. Selection of wavelength and time ranges. Analyst, The, 2001, 126, 1135-1141.	1.7	2
121	Simultaneous multiwavelength spectrophotometric determination of 1:2 metalâ€complex dyes for leather. Coloration Technology, 1995, 111, 199-202.	0.1	1
122	Use of indirect multiple linear regression for multicomponent dye analysis in a leather tanning bath. Coloration Technology, 1997, 113, 311-316.	0.1	1
123	Aza-Michael reaction with enone-modified vegetable oils: evidence of the keto–enolic equilibrium by NIR chemical imaging and evolving factor analysis. Analytical and Bioanalytical Chemistry, 2011, 399, 1975-1982.	1.9	1
124	Robust freeze-drying process re-design of a legacy product based on risk analysis and design of experiments. Drug Development and Industrial Pharmacy, 2020, 46, 2022-2031.	0.9	1
125	4-(8-Quinolylazo)-1-Aminonaphtalene as a Metallochromic Indicator for Cu(II), Ni (II) and Hg(II). Analytical Letters, 1984, 17, 1009-1023.	1.0	0