



CAPÍTULO 4

Referencias Bibliográficas

REFERENCIAS BIBLIOGRÁFICAS

Analytical Methods Committee (1994). Analytical Division, The Royal Society of Chemistry. *Analyst.*, 119: 2363–2366.

Araujo, P.W. y Brereton, R.G. (1996). Experimental design. I. Screening. *Trends Anal. Chem.*, 15: 26-31.

Araujo, P.W. y Brereton, R.G. (1996). Experimental design. II. Optimization. *Trends Anal. Chem.*, 15: 63-70.

Araujo, P.W. y Brereton, R.G. (1996). Experimental design. III. Quantification. *Trends Anal. Chem.*, 15: 156-163.

Ashy, A.R.; El Sayed, Y.M.; Islam, S.I. (1986). Comparison of fluorescence polarization immunoassay and high-performance liquid chromatography for the quantitative determination of phenytoin, phenobarbitone and carbamazepine in serum. *J. Pharm. Pharmacol.* 38: 572-577.

Barros Neto B., Scarminio I.S., Bruns R.E. (2001). *Como fazer experimentos*, Editora da Unicamp, Campinas.

Bautista, R.D.; Jimenez, A.I.; Jimenez, F.; Arias, J.J. (1996). Resolution of ternary and quaternary mixtures of drugs in pharmaceutical preparations by use of spectrophotometric data in conjunction with PLS-1 and PLS-2 data processing methods. *Anal. Lett.*, 29: 2645-2665.

Berger, A.J., Koo, T., Itzkan, I. y Feld, M.S. (1998). An enhanced algorithm for linear multivariate calibration. *Anal. Chem.*, 70: 623-627.

Bezemer, E.; Rutan, S.C. (2002). Three-way alternating least squares using three-dimensional tensors in MATLAB. *Chemom. Intell. Lab. Syst.*, 60: 239-251.

Bhatti, M.M.; Hanson, G.D.; Schultz, L. (1998). Simultaneous determination of phenytoin, carbamazepine, and 10,11-carbamazepine epoxide in human plasma by high-performance liquid chromatography with ultraviolet detection. *J. Pharm. Biom. Anal.*, 16: 1233-1240.

Booksh, K.S. y Kowalski, B.R. (1994). Theory of analytical chemistry. *Anal. Chem.*, 66: 782A-791A.

Booksh, K.S.; Kowalski, B.R. (1994). Comments on the DATA ANALYSIS (DATAN) algorithm and rank annihilation factor analysis for the analysis of correlated spectral data. *J. Chemom.*, 8: 287-292.

Bowers, L.D. (1998). Analytical goals in therapeutic drug monitoring. *Clin. Chem.*, 44: 375-380.

BP (1998). British Pharmacopeia, CD version 2.0. The Stationary Office Ltd. Norwich

Brereton, R.G. (1990). *Chemometrics. Applications of the Mathematics and Statistics to Laboratory Systems*, Ellis Horwood.

Bro, R. (1998). *Multi-way analysis in the food industry. Models, algorithms, and applications*. PhD thesis, University of Amsterdam (NL).

Brown, S.D. (1991). Rapid parameter estimation with incomplete chemical calibration models. *Chemom. Intell. Lab. Syst.*, 10: 87-105.

Carroll, J.D.; Chang, J. (1970). Analysis of individual differences in multidimensional scaling via an N-way generalization of "Eckart-Young" decomposition. *Psychometrika*, 35: 283-319.

Centner, V.; de Noord, O.E.; Massart; D.L. (1998). Detection of nonlinearity in multivariate calibration. *Anal. Chim. Acta*, 376: 153-168.

Centner, V.; Massart, D.L (1998). Optimization in locally weighted regression. *Anal. Chem.*, 70: 4206-4211.

Chelberg, R.D.; Gunawan, S.; Treiman, D.M. (1988). Simultaneous high-performance liquid-chromatographic determination of carbamazepine and its principal metabolites in human plasma and urine. *Ther. Drug Monit.*; 10: 188-193.

Chen, M.; Zhang, X.; Shao, Q.; Gan, L.(1991). Analysis of dexamethasone sodium phosphate injection by UV-spectrophotometry. *Yaowu. Fénix Zazhi*, 11: 103-104.

Clayton, C.; Hines, J.; Elkins, P. (1987). Detection limits with specified assurance probabilities. *Anal. Chem.*, 59: 2506-2514.

Collado, M. S.; Mantovani, V. E.; Goicoechea, H. C.; Olivieri, A. C. (2000). Simultaneous spectrophotometric-multivariate calibration determination of several components of ophthalmic solutions; phenylephrine, chloramphenicol, antipyrine, methylparaben and thimerosal. *Talanta*, 5 (52): 909-920.

Collado, M.S.; Satuf, M.L.; Goicoechea, H.C.; Olivieri, A.C. (2002). Complementary use of partial least-squares and artificial neural networks for the non-linear spectrophotometric analysis of pharmaceutical samples. *Anal. Bioanal. Chem.*, 374: 460-465.

Compañó Beltrán, R.; Rios Castro, A. (2002). *Garantía de calidad en los laboratorios analíticos*. Ed. Síntesis, Madrid.

Culzoni, M.J.; Goicoechea H.C.; Bearzoti, M.; Cabezón M. y Olivieri A. (2006). 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. *Analyst*, 131: 718 - 723.

Currie, L. (1995). Recommendations in Evaluation of Analytical Methods including Detection and Quantification Capabilities. *Pure Appl. Chem.*, 67: 1699-1723.

Currie, L. (1999). Detection and quantification limits: origins and historical perspective. *Anal. Chim. Acta*, 391:127-134.

Damiani, P.; Escandar, G.; Olivieri, A.; Goicoechea, H. (2005). "Multivariate calibration: a powerful tool in pharmaceutical analysis". *Curr. Pharm. Anal.*, 1: 145-154.

Damiani, P.; Nepote, A.; Bearzotti, M.; Olivieri, A.C. (2004). A test field for the second-order advantage in bilinear least-squares and parallel factor analyses: fluorescence determination of ciprofloxacin in human urine. *Anal. Chem.*, 76: 2798-2809.

Damiani, P.; Borraccetti, M.; Olivieri, A.. (2002). Direct and simultaneous spectrofluorimetric determination of naproxen and salicylate in human serum assisted by chemometric analysis. *Anal. Chim. Acta*, 471: 87-96.

Danzer, K.; Currie, L. (1998). Guidelines for calibration in analytical chemistry. Part. 1. Fundamentals and single component calibration. *Pure Appl. Chem.*, 70: 993-1014.

Das, B.; Chatterjee, S.K.; Das, S.K. (1986). Thin-layer chromatographic method for rapid identification and quantification of corticosteroid sodium phosphates in pharmaceutical preparations. *J. Liq. Chromatogr.*, 9: 3461 – 3467.

Das-Gupta, A.; Vega, A.; Wells, A.; Datta, P. (1999). Effect of heating human sera at a temperature necessary to deactivate human immunodeficiency virus on measurement of free phenytoin, free valproic acid, and free carbamazepine concentrations. *Ther. Drug Monit.*, 21: 421-425.

Das-Gupta, V. (1979). Quantitative dexamethasone and dexamethasone sodium phosphate determinations in pharmaceutical dosage forms by high-pressure liquid chromatography. *J. Pharm. Sci.*, 68: 926-928.

Datta, K.; Das, S.K. (1993). Densitometric quantification of corticosteroid sodium phosphate salts in parenteral preparations or eye and ear drops after reverse-phase ion-pair TLC. *J. Planar Chromatog. Mod. TLC*, 6: 204 - 207.

Deming, S.; Morgan, S. (1973). Simplex Optimization of Variables. *Anal. Chem.*, 45: 278-282.

Despagne, F.; Massart, D.L. (1998). Neural networks in multivariate calibration. *Analyst*, 123: 157R-178R.

de-Wasch, K; de-Brabander, H.F.; van de-lele, M.; Vercammen, J; Courtheyn, D; Impens, S; (2000). Differentiation between dexamethasone and betamethasone in a mixture using multiple mass spectrometry. *J Chromatogr, A* 926(1): 79-86.

Escandar, G.M.; González Gómez, D.; Espinosa Mansilla, A.; Muñoz de la Peña, A.; Goicoechea, H.C. (2004). Determination of carbamazepine in serum and pharmaceutical preparations using immobilization on a nylon support and fluorescent detection. *Anal. Chim. Acta*, 506: 161-170.

Espinosa-Mansilla, A.; Durán-Merás, I.; Galián, R. (2001). Simultaneous fluorimetric determination of pteridine derivatives: comparison between synchronous, partial least-squares, and hybrid linear analysis methods. *Appl. Spectrosc.*, 55: 701-707.

EURACHEM (1998). *The fitness for Purpose of Analytical Methods. A Laboratory Guide to Method Validation and Related Topics*. EURACHEM Secretariat, Teddington, Middlesex.

Faber, N. M.; Ferré, J.; Boqué, R.; Kalivas, J.H. (2002). Second-order bilinear calibration: the effects of vectorising the data matrices of the calibration set. *Chemom. Intell. Lab. Syst.*, 63: 107-116.

Faber, N.M. (2000). Exact presentation of multivariate calibration model as univariate calibration graph. *Chemom. Intell. Lab. Syst.*, 50: 107-114.

Faber, N.M. (2001). The price paid for the second-order advantage when using the generalized rank annihilation method. *J. Chemom.*, 15: 743-748.

Faber, N.M. (2002). Towards a rehabilitation of the generalized rank annihilation method (GRAM). *Anal. Bioanal. Chem.*, 372: 683-687.

Fadnavis, N.; Bhaskar, V.; Deshpande, A.; Bhalerao, U. (2001). Determination of enantiomeric excess of dextropropoxyphene and α -(+) oxyphene by chiral high-performance liquid chromatography. *Anal. Chim. Acta*, 441: 297-301.

Ferré, J.; Boqué, R.; Fernández Band, B.; Larrechi, M.S.; Rius, F.X. (1997). Figures of merit in multivariate calibration. Determination of four pesticides in water by flow injection analysis and spectrophotometric detection. *Anal. Chim. Acta*, 348:167-175.

Ferré, J.; Faber, N.M. (2003). Net analyte signal calculation for multivariate calibration. *Chemom. Intell. Lab. Syst.*, 69: 123-136.

Franceschi, L.; Furlanut, M. (2005). A simple method to monitor plasma concentration of oxcarbamazepine, carbamazepine, their main metabolites and lamotrigine in epileptic patients. *Pharmacol. Res.*; 51: 297-302.

Gagne, D.; Lodge, BA. (1980). Analysis of dexamethasone sodium phosphate formulations by high-performance liquid chromatography. *J. Chromatography*, 193: 160-162.

Galeano Diaz, T.; Guiberteau, A.; Ortiz Burguillos, J.M.; Salinas, F. (1997). Comparison of chemometric methods: derivative ratio spectra and multivariate methods (CLS, PCR and PLS) for the resolution of ternary mixtures of the pesticides carbofuran carbaryl and fenamiphos after their extraction into chloroform. *Analyst*, 122: 513-517.

Galera, M.M.; Zamora, D.P.; Vidal, J.L.M.; Frenich, A.G.; Espinosa Mansilla, A.; Munoz de la Pena, A.; López, F.S. (2003). Determination of carbendazim, thiabendazole and fuberidazole using a net analyte signal-based method. *Talanta*, 59: 1107-1116.

García, E.; García, A.; Barbas, C. (2001). Validated HPLC method for quantifying permethrin in pharmaceutical formulations. *J. Pharm. Biomed Anal.*, 24: 999

Garrido Frenich, A.; Picon Zamora, D.; Martínez Galera, M.; Martínez Vidal, J.L. (2003). Application of GRAM and TLD to the resolution and quantitation of real complex multicomponent mixtures by fluorescence spectroscopy. *Anal. Bioanal. Chem.*, 375: 974-980.

Gemperline, P.J.; Long, J.R.; Gregoriou, V.G. (1991). Non-linear multivariate calibration using principal components regression and artificial neural networks. *Anal. Chem.*, 63: 2313-2323.

Gerritsen, M.J.P.; Tanis, H.; Vandeginste, B.G.M.; Kateman, G. (1992). Generalized rank annihilation factor analysis, iterative target transformation factor analysis, and residual bilinearization for the quantitative analysis of data from liquid chromatography with photodiode array detection. *Anal. Chem.*, 64: 2042-2056.

Goicoechea, H.C.; Muñoz de la Peña, A.; Olivieri, A.C. (1999). Determination of theophylline in blood serum by UV spectrophotometry and partial least-squares (PLS-1) calibration. *Anal. Chim. Acta*, 384: 95-103.

Goicoechea, H.C.; Olivieri, A. C. (2001). A comparison of orthogonal signal correction and net analyte preprocessing methods. Theoretical and experimental study. *Chemom. Intell. Lab. Syst.*, 56: 73-81.

Goicoechea, H.C.; Olivieri, A.C. (1999). Enhanced synchronous spectrofluorimetric determination of tetracycline in blood serum by chemometric analysis. Comparison of partial least-squares and hybrid linear analysis calibrations. *Anal. Chem.*, 71: 4361-4368.

Goicoechea, H.C.; Olivieri, A.C. (2000). MULTIVAR. A program for multivariate calibration incorporating net analyte signal calculations. *Trends Anal. Chem.*, 19: 599-605.

González, A.; Herrador, M.; Asuero, A. (1999). Intra-laboratory testing of method accuracy from recovery assays. *Talanta*, 48: 729-736.

Goodman Gilman, A.; Hardman, J.G.; Limbrid, L.E. (2001). *Goodman & Gilman's the Pharmacological Basis of Therapeutics*, 10th ed., Mc. Graw Hill, New York.

Goodman Hilman, A., Rall, T., Nier, A. y Taylor, P. (1996). *Las bases farmacológicas de la terapéutica*, 9º ed., Ed. McGraw-Hill Interamericana, México.

Goodman Hilman, A., Rall, T., Nier, A. y Taylor, P. (1996). *Las bases farmacológicas de la terapéutica*, 9º ed., Ed. McGraw-Hill Interamericana, México.

Green, J.M. (1996). A practical guide to analytical method validation, *Anal. Chem.*, 68: 305A-309A.

Haaland, D.M. y Thomas, E.V. (1988). Partial least-squares methods for spectral analyses. 1. Relation to other quantitative calibration methods and the extraction of qualitative information. *Anal. Chem.*, 60: 1193-1202.

Haaland, D.M. y Thomas, E.V. (1988). Partial least-squares methods for spectral analyses. 2. Application to simulated and glass spectral data. *Anal. Chem.*, 60: 1202-1208.

Haaland, D.M. y Thomas, E.V (1988). Partial least-squares methods for spectral analyses. 3. Quantitative infrared analysis of borophosphosilicate films using multivariate statistical methods. *Anal. Chem.*, 60: 1208-1217.

Haaland, D.M.; Han, L.; Niemczyk, T.M. (1999). Use of CLS to understand PLS IR calibration for trace detection of organic molecules in water. *Appl. Spectrosc.*, 53: 390-395.

Hadjiiski, L.; Geladi, P.; Hopke, P. (1999). A comparison of modeling nonlinear systems with artificial neural networks and partial least squares. *Chemom. Intell. Lab. Syst.*, 49: 91-103.

Harshman, R.A. (1970). Foundations of the PARAFAC procedure: model and conditions for an explanatory multi-mode factor analysis. *UCLA Work. Pap. Phon.*, 16: 1-84.

Hart, S.J.; Hall, G.J.; Kenny, J.E. (2002). A laser-induced fluorescence dual-fibre optic array detector applied to the rapid HPLC separation of polycyclic aromatic hydrocarbons. *Anal. Bioanal. Chem.*, 372: 205-215.

Hartley, R.; Lucock, M.; Cookman, J.R.; Becker, M.; Forsythe, W.I. (1986). High-performance liquid-chromatographic determination of carbamazepine and carbamazepine 10,11-epoxide in plasma and saliva following solid-phase sample extraction. *J. Chromatogr.*, 380: 347-356.

He, J.; Shibukawa, A.; Nakagawa, T.(1992). High-performance frontal analysis - high-performance liquid-chromatographic system for stereoselective determination of unbound ketoprofen enantiomers in plasma after direct sample injection. *J. Pharm. Biom. Anal.*, 10: 289-294.

Hortwitz, W. (1982). Evaluation of analytical methods used for regulation of food and drugs. *Anal. Chem.*, 54: 67A.

Hruschka, W.R.; Norris, K. (1982). Least squares curve fitting of near infrared spectra predicts protein and moisture content of ground wheat. *Appl. Spectrosc.*, 36: 261-265.

ICH Harmonised Tripartite Guideline (1996)Topic Q2B: *Validation of Analytical Procedures: Methodology*, CPMP/ICH/281/95, Step 4.

ISO (1993). *International Organization for Standardization, Statistics, Vocabulary and symbols*. ISO 3534-1, ISO, Geneva.

ISO/IEC 17025 (1999), *Requisitos generales para la competencia de los laboratorios de ensayo y de calibración*. IRAM 301:2000.

Jochum, C.; Jochum, P.; Kowalski, B.R. (1981). Error propagation and optimal performance in multicomponent analysis. *Anal. Chem.*, 53: 85-92.

Kaplan, L.A., Pesce, A.J. (1986). *Química clínica: técnicas de laboratorio, fisiopatología y métodos de análisis*, Ed. Médica Panamericana, Buenos Aires.

Kasabov, N.K. (1998), *Foundation of neural networks, fuzzy systems and knowledge engineering*, The MIT PRESS, Cambridge.

Kazemipour, M.; Noroozian, E.; Saber Tehrani, M.; Mahmoudian, M. (2002). A new second-derivative spectrophotometric method for the determination of permethrin in shampoo. *J. Pharm. Biomed Anal.*, 30: 1379-1384.

Kellner, R.; Mermet, J. M.; Otto, M.; Widmer, H. M. (1998). *Analytical Chemistry. The Approved Text to the FECS Curriculum Analytical Chemistry*, Wiley-VCH, Weinheim.

Kennard, R.W.; Stone, L.A. (1969). Computer aided design of experiments. *Technometrics*, 11: 137-148.

Korany, M.A.; Elsayed, M.A.; Mahgoub, H.; Korany, E. (1990). Computer-assisted spectrophotometry: multicomponent analysis with a discrete Fourier transform. *Talanta*, 37: 1183-1188.

Korpela, M.T.; Kurittu, J.S.; Karvinen, J.T. y Karp, M.T. (1998). A recombinant escherichia coli sensor strain for the detection of tetracyclines. *Anal. Chem.*, 70: 4457-4462.

Kröse, B.; van der Smagt, P. (1996), *An introduction to neural networks*, University of Amsterdam, Amsterdam.

Lancas, F.M.; Sozza, M.A.; Queiroz, M.E.C. (2003). [Simultaneous plasma lamotrigine analysis with carbamazepine, carbamazepine 10,11 epoxide, primidone, phenytoin, phenobarbital, and PEMA by micellar electrokinetic capillary chromatography \(MECC\)](#). *J. Anal. Toxicol.*; 27: 304-308.

Lee, S.H.; Li, M.; Suh, J.K. (2003). Determination of carbamazepine by chemiluminescence detection using chemically prepared tris(2,2'-bipyridine)ruthenium(III) as oxidant. *Anal. Sci.*, 19: 903-906.

Lemus Gallego, J. M.; Perez Arroyo, J. (2001). Micellar electrokinetic capillary chromatography as an alternative method for the determination of dexamethasone, trimethoprim and polymyxin B. *Fresenius' J Anal Chem*, 370(7): 973-975.

Lemus Gallego, J.M.; Perez Arroyo, J. (2001). Simultaneous resolution of dexamethasone and polymyxin B by spectrophotometry derivative and multivariate methods. *Anal Lett*, 34(8):1265-1283.

Liang, Y.; Kvalheim, O.M.; Keller, H.R.; Massart, D.L.; Kiechle, P.; Erni, F. (1992). Heuristic involving latent projections: resolving two-way multicomponent data. Detection and resolution of minor constituents. *Anal. Chem.*, 64: 946-953.

Lindberg, W.; Ohman, J.; Wold, S. (1986). Multivariate resolution of overlapped peaks in liquid chromatography using diode-array detection. *Anal. Chem.* 58: 299-303.

Linder, M.; Sundberg, R. (1998). Second-order calibration: bilinear least squares regression and a simple alternative. *Chemom. Intell. Lab. Syst.*, 42: 159-178.

Linder, M.; Sundberg, R. (2002). Precision of prediction in second-order calibration, with focus on bilinear regression methods. *J. Chemom.*, 16: 12-27.

Liu, K. R.; Chen, S. H.; Kou, H. S.; Wu, H. L. (1994). High performance liquid chromatographic determination of betamethasone and dexamethasone. *J. Chromatogr, A* 675(2):455-460.

Lorber, A. (1984). Validation of hypothesis on a data matrix by target factor analysis. *Anal. Chem.*, 56: 1004-1010.

Lorber, A.; Kowalski, B.R. (1990). Alternatives to cross-validated estimation of the number of factors in multivariate calibration. *Appl. Spectrosc.*, 44: 1464-1470.

Luis, M.L.; Fraga, J.M.G.; Jiménez, F.; Jiménez, A.I.; Arias, J.J. (2001). Simultaneous spectrophotometric determination of diuretics by using multivariate calibration methods. *Talanta*, 53: 761-770.

Marbach, R.; Heise, H.M. (1990). Calibration modelling by partial least-squares and principal component regression and its optimization using an improved leverage correction for prediction testing. *Chemom. Intell. Lab. Syst.*, 9: 45-63.

Marsili, N. R.; Lista, A.; Fernandez Band, B. S.; Goicoechea, H. C. y Olivieri, A. C. (2004). New method for the determination of benzoic and sorbic acids in commercial orange juice based on second-order spectrophotometric data generated by a pH gradient flow injection technique. *J. Agric. Food Chem.*, 52: 2479-2484.

Marsili, N. R.; Lista, A.; Fernandez Band, B. S.; Goicoechea, H. C. y Olivieri, A. C. (2005) Evaluation of complex spectral-pH three-way arrays by modified bilinear least-squares: determination of four different dyes in interfering systems. *Analyst*, 130: 1291-1298.

Martens, H.; Izquierdo, L.; Thomassen, M.; Martens, M. (1986). Partial least-squares regression on design variables as an alternative to analysis of variance. *Anal. Chim. Acta.*, 19: 133-148.

Martens, H.; Naes, T. (1989). *Multivariate Calibration*, Ed. John Wiley & Sons, New York.

Martindale, W.(1993). *The extra pharmacopeia*. 30th Ed., The Pharmaceutical Press, London.

Massart, D.J.; Vandegisnte, B.G.M.; Buydens, L.M.C; De Jong, S.; Lewi, P.J. y Smeyers-Verbeke, J. (1997) *Handbook of Chemometrics and Qualimetrics: A and B*, Ed. Elsevier, Amsterdam.

MATLAB 5.3 (1999). Matrix computation laboratory. The Math Works Inc., Natick, Massachusetts, USA.

Maurí Aucejo, A.R.; Llobat Estellés, M.; Marín Saez, R.; San Martín Cigés, M.D.; Alvarez Alonso, C. (1993). Apparent content curves: new analytical applications. *Fresenius J. Anal. Chem.*, 346: 888-895.

McWhinney, B. C.; Ward, G; Hickman, P. E. (1996). Improved HPLC method for simultaneous analysis of cortisol, 11-deoxycortisol, prednisolone, methylprednisolone, and dexamethasone in serum and urine. *Clin-Chem* (Washington, DC), 42(6): 979-981.

Miller J.C y Miller J.N. (1993). *Estadística para la química analítica* Addison-Wesley Iberoamerican S.A.

Montgomery D.C. (1991). *Diseño y análisis de experimentos*, Ed. Grupo Editorial Iberoamérica, México.

Morgan E. (1995). *Chemometrics: Experimental Design*. John Wiley & Sons, Chichester.

Munoz de la Peña, A.; Espinosa Mansilla, A.; Valenzuela, M.I.A; Goicoechea, H.C.; Olivieri, A.C. (2002). Comparative study of net analyte signal-based methods and partial least squares for the simultaneous determination of amoxicillin and clavulanic acid by stopped-flow kinetic analysis. *Anal. Chim. Acta*, 463: 75-88.

Myers, R.H.; Montgomery, D.C. (1995). *Response surface methodology. Process and product optimization using designed experiments*. John Wiley & Sons, Inc, New York.

Naes, T.; Martens, H. (1998). Principal component regression in NIR [near-infra-red] analysis: viewpoints, background details and selection of components. *J. Chemom.*, 2: 155-167.

Olivieri, A. (2005). On a versatile second-order multivariate calibration method based on partial least-squares and residual bilinearization: Second-order advantage and precision properties. *J. Chemom.*, 19: 253-265

Olivieri, A.; Faber, N.; Ferré, J.; Boqué, R.; Kalivas, J.; Mark, H. (2006). Uncertainty Estimation and Figures of Merit for Multivariate Calibration (IUPAC Technical Report). *Pure Appl. Chem.*, 78: 633-661.

Olivieri, A.C.; Goicoechea, H.C.; Iñón, F.A. (2004). MVC1: An integrated MATLAB toolbox for first-order multivariate calibration. *Chemom. Intell. Lab. Syst.*; 72: 189-197.

Osten, D.W.; Kowalski, B.R. (1984). Multivariate curve resolution in liquid chromatography. *Anal. Chem.*, 56: 991-995.

Paatero, P. (1994). Positive matrix factorization: a non negative factor model with optimal utilization of error estimates of data values. *Sci. Total. Environ.*, 5: 111-116.

Paatero, P. (1997). A weighted non-negative least squares algorithm for three-way "PARAFAC" factor analysis. *Chemom. Intell. Lab. Syst.*, 38: 223-242.

R. Fletcher (1980). *Practical methods for optimization*, Vol 1: Unconstrained optimization, Wiley, New York.

Raggi M.A.; Casamenti, G.; Mandrioli, R.; Sabbioni, C.; Volterra, V. (2000). A rapid LC method for the identification and determination of CNS drugs in pharmaceutical formulations. *J. Pharm. Biom. Anal.*; 23: 161-167.

Raggi, M.A.; Casamenti, G.; Mandrioli, R., Sabbioni, C.; Volterra V. (2000). A rapid LC method for the identification and determination of CNS drugs in pharmaceutical formulations. *J. Pharm. Biom. Anal.*; 23: 161-167.

Ramis Ramos, G, y García Álvarez Coque, M. C. (2002). *Quimiometría, Calibración y Regresión Lineal*. Editorial Síntesis S. A., Madrid.

Rezaei, Z.; Hemmateenejad, B.; Khabnadideh, S.; Gorgin, M. (2005). Simultaneous spectrophotometric determination of carbamazepine and phenytoin in serum by PLS regresión and comparison Ruth HPLC. *Talanta*; 65: 21

Riu, J.; Rius, F. (1996). Assessing the accuracy of analytical methods using linear regresión with errors in both axes. *Anal. Chem.*, 68: 1851-1857.

Rumelhart, D.E.; McClelland, J.L. (1986). *Parallel distributed processing*, MIT Press, Cambridge.

Russel, S.; Norvig, P. (1996), *Inteligencia artificial. Un enfoque moderno*, 1ra ed., Ed. Prentice may Hispanoamericana S. A., México.

Sánchez, A.; Garcia, R.; Abadin, J.A.; Duran, J.A. (1999). Determination of free serum carbamazepine by protein precipitation with sulfosalicylic acid. *Pharm. Pharmacol. Commun.*, 5: 435-438.

Sánchez, A.; Garcia, R.; Abadin, J.A.; Duran, J.A. (1999). Determination of free serum carbamazepine by protein precipitation with sulfosalicylic acid. *Pharm. Pharmacol. Commun.*, 5: 435-438.

Sanchez, E.; Kowalski, B.R. (1986). Generalized Rank Annihilation Factor Analysis. *Anal. Chem.*, 58: 496-499.

Santos Montes, A.; Gasco López, M. I.; Izquierdo Hornillos, R. (1994). Simultaneous determination of dexamethasone and betamethasone in pharmaceuticals by reversed-phase HPLC. *Chromatographia*, 39(9-10):539-542.

Sanz, J.; Pérez, M.; Martínez, M.T.; Plaza, M. Experimental design methodologies to optimize monobutyltin chloride determination by hydride generation gas phase molecular absorption spectrometry. *Talanta*, 50:149-164

Saurina, J. (2000). Analytical application of pH-gradients in flow-injection analysis and related techniques. *Rev. Anal. Chem.*, 19: 157-178.

Saurina, J.; Leal, C.; Compano, R.; Granados, M.; Tauler, R.; Prat, M.D. (2000). Determination of triphenyltin in sea water by excitation-emission matrix fluorescence and multivariate curve resolution. *Anal. Chim. Acta.*, 409: 237-245.

Scheffé, H. (1958). Experiments with mixtures. *J. R. Stat. Soc.*, B20 (2): 344-360.

Sekulic, S.; Seasholtz, M.B.; Wang, Z.; Kowalsky, B.R.; Lee, S.E.; Holt, B.R (1993). Nonlinear multivariate calibration methods in analytical chemistry. *Anal. Chem.*, 65: 835A-845A.

Sena, M.M; Chaudhry, Z.F; Collins, C.H; Poppi, R.J. (2004). Direct determination of diclofenac in pharmaceutical formulations containing B vitamins by using UV spectrophotometry and partial least squares regression. *J. Pharm. Biomed. Anal.*, 36: 743-749.

Shaffer, R.E.; Small, G.W. (1997). Learning optimisation from nature. Genetic algorithms and simulated annealing. *Anal. Chem.*, 69: 236A-242A.

Shaw, L.M. (1998). Therapeutic drug monitoring: new drugs expand testing range. *Clin. Lab. News*, 24: 10-12.

Skoog, A.D. y Leary, J. (1994). *Análisis instrumental*, 4º ed, Ed. McGraw Hill, Buenos Aires.

Strange, R.S. (1990). Introduction to Experiment Design for Chemists. *J. Chem. Ed.*, 67: 113-115.

Swartz, M.; Krull, I. (2003). Validation of Bioanalytical Methods-Highlights of FDA's Guidance. *LCGC North America*, 21: 137-140.

Talski, G. (1994). *Derivate spectrophotometry. Low and higher order*. Editorial VCH, Cambridge, UK.

Thomas, E.V. (1994). A primer on multivariate calibration. *Anal. Chem.*, 66: 795 A-804 A.

Thompson, M.; Ellison, S.; Wood, R. (2002). Harmonized Guidelines for Single-Laboratory Validation of Methods of Analysis (IUPAC Technical Report). *Pure Appl. Chem.*, 74: 835-855.

Toasaksiri, S.; Massart, D.L.; Vander-Heyden Y. (2000). Study of method validation criteria in a capillary electrophoresis method for the separation of non-steroidal anti-inflammatory drugs. *Anal.Chim. Acta.* , 416: 29-42.

USP XXIV (2000). United States Pharmacopeia XXIV , United States Pharmacopeial Convention, Rockville, MD.

USP–NF 25. (2000) *Validation of compendial methods*.

Valcárcel, M. (1999). *Principios de Química Analítica*. Ed. Springer-Velay Ibérica, Madrid.

Vander Heyden, Y.; Nijhuis, A.; Smeyers-Verbeke, J.; Vandeginste, B.G.M.; Massart, D.L. (2001). Guidance for robustness/ruggedness test in method validation. *J. Pharm. Biomed Anal.*, 24:723-753.

Vanderlinde, R.E.; Kowalski, P.(1971). The clinical biochemistry of phosphorus. *Clin. Biochem.*, 4: 76-88

Wang, Z.; Luo, G.O.; Zhou, G.; Yao, C. (1989).Application of PLS [partial least-squares] method in simultaneous spectrophotometric determination of trace metal ions. *Fenxi. Huaxue*, 17: 317-320.

Werbos, P. (1982). *Applications of Advances in Nonlinear Sensitivity Analysis, in System Modeling and Optimization: Proc. of the Int. Federation for Information Processes*. Eds.: R. Drenick, F Kozin, Springer Verlag, New York, USA.

Wise, B.M.; Gallagher, N.B.; Martin, E.B. (2001). Application of PARAFAC2 to fault detection and diagnosis in semiconductor etch. *J. Chemom.*, 15: 285-298.

Wold, S. (1992), Nonlinear partial least squares modelling. II. Spline inner relation. *Chemom. Intell. Lab. Syst.*, 14:71-84.

Wu, M.L.; Li, B.X.; Zhang, Z.J. (2001). Flow-injection chemiluminescence determination of sodium phosphate dexamethasone using online electrogenerated cobalt(III) as oxidant. *Fenxi-Huaxue*, 29(3): 267-270.

Wu, S. M.; Wu, H. L.; Chen, S. H. (1995). Determination of betamethasone and dexamethasone in plasma by fluorogenic derivatization and liquid chromatography. *Anal Chim Acta*, 307(1): 103-107.

Xi, M.; Yang, Y.; Shao, Q.; Peng, Y. (1991). Differential- spectrometric determination of dexamethasone sodium phosphate injection. *Yaowu. Fénix Zazhi*, 11: 291-292.

Xie, Y.L.; Baeza Baeza, J.J.; Ramis Ramos, G. (1996). Second-order tensorial calibration for kinetic spectrophotometric determination. *Chemom. Intell. Lab. Syst.*, 32: 215-232.

Xie, Y.L.; Hopke, P.K.; Paatero, P. (1998). Positive matrix factorization applied to a curve resolution problem. *J. Chemom.*, 12: 357-364.

Xu, L. y Schechter, I. (1997). A calibration method free of optimum factor number selection for automated multivariate analysis. Experimental and theoretical study. *Anal. Chem.*, 69: 3722-3730.

Xu, L.; Schechter, I. (1996). Wavelength selection for simultaneous spectroscopic analysis. Experimental and theoretical study. *Anal. Chem.*, 68(14): 2392-2400.

Yao, X.; Qiao, Z. (1988). Assay of dexamethasone sodium phosphate injection by reverse-phase HPLC. *Yiao. Gongye*, 19: 172-173.

Zupan, J. ; Gasteiger J. (1999), *Neural networks in chemistry and drug design*, Second Edition, Ed. Wiley-VCH, Weinheim.