

## **PUBLICACIONES CIENTÍFICAS 2014**

### **GRUPO DE BIOSENSORES ANALÍTICOS (GBA)**

#### **Spectrally marched upconverting luminescent nanoparticles for monitoring enzymatic reactions.**

S. Wilhelm, M. Del Barrio, J. Heiland, S.F. Himmelstoß, J. Galbán, O. Wolfbeis, T. Hirsch (GBA)  
ACS Applied Materials & Interfaces, 6, 15427-15433 (2014)

#### **Enzyme-Induced modulation of the emission of upconverting nanoparticles: Towards a new sensing scheme for glucose.**

M. del Barrio, S. de Marcos, V. Cebolla, J. Heillan, S. Wilhem, T. Hirsch, J. Galbán (GBA)  
Biosensors and Bioelectronic, 59, 14-20 (2014)

#### **Analytical applications of the optical properties offerric hemoglobin: a theoretical and experimental study.**

V. Sanz, S de Marcos, J Galbán (GBA)  
Microchemical Journal, 114, 175-171 (2014)

#### **An optical sensor for pesticide determination based on the autoindicating optical properties of prooxidase.**

S. de Marcos, E. Callizo, E. Mateos, J. Galbán (GBA)  
Talanta, 122, 251-256 (2014)

### **GRUPO DE ESPECTROSCOPIA ANALÍTICA Y SENSORES (GEAS)**

#### **Detection and characterization of silver nanoparticles and dissolved species of silver in culture medium and cells by AsF<sub>6</sub>-FFF-UV-Vis-ICPMS: application nanotoxicity tests.**

E. Bolea, J. Jiménez-Lamana, F. Laborda, I. Abad, C. Blade, L. Arola, J.R. Castillo (GEAS)  
Analyst, 139, 914-922 (2014)

#### **Single particle inductively coupled plasma mass spectrometry: A powerful tool for nanoanalysis.**

F. Laborda, E. Bolea, J. Jiménez-Lamana (GEAS)  
Analytical Chemistry, 86(5), 2270-2278 (2014)

#### **Silver nanoparticle detection and characterization in silver colloidal products using screen printed electrodes.**

G. Cepriá, W. R. Córdova, J. Jiménez-Lamana, F. Laborda, J. R. Castillo (GEAS)  
Analytical Methods, 6(9), 3072–3078 (2014)

#### **Suitability of the voltammetry of immobilized microparticles to detect and discriminate lead compounds in microsamples of ancient black cosmetics.**

J. Pérez-Arantegui, G. Cepriá (GEAS)  
Electrochimica Acta, 138, 247-255 (2014)

#### **Chemical halide vaporization as a sample introduction technique for atomic spectroscopy: significance of its kinetic mechanism.**

A. López-Molinero, D. Sipiera, J.R. Castillo (GEAS)  
Journal of Analytical Atomic Spectrometry, 29, 111-121 (2014)

#### **General Procedure for the Easy Calculation of pH in an Introductory Course of General or Analytical Chemistry.**

G. Cepriá, L. Salvatella (GEAS)

Journal of Chemical Education, 91(4), 524-530 (2014)

**An insight into silver nanoparticles bioavailability in rats.**

J. Jiménez-Lamana, F. Laborda, E. Bolea, I. Abad, J. R. Castillo, J. Bianga; M. He, K. Bierla, S. Mounicou, L. Ouerdane, S. Gaillet, J.M. Rouanet, J. Szpunarb (GEAS)  
Metallomics, 6, 2242-2249 (2014)

**Field-Emission Scanning Electron Microscopy and Energy-Dispersive X-Ray Analysis to Understand the Role of Tannin-Based Dyes in the Degradation of Historical Wool Textiles.**

A. Restivo, I. Degano, E. Ribechini, J. Pérez-Arantegui, M.P. Colombini (GEAS)  
Microscopy and Microanalysis, 20, 1534-1543 (2014)

**Spread and partitioning of arsenic in soils from a mine waste site in Madrid province (Spain).**

M.A. Gómez-González, S. Serrano, F. Laborda, F. Garrido (GEAS)  
Science of the Total Environment, 500-501, 23-33 (2014)

**GRUPO UNIVERSITARIO DE INVESTIGACIÓN ANALÍTICA (GUIA)**

**Seveso Disaster and the European Seveso Directives.**

C. Nerín, B. Seco, A. Tena, M. Calvo (GUIA)  
Encyclopedia of Toxicology (3rd edition), vol. 4, pp. 244-247. Ed. P. Wexler. Elsevier Inc. Academic Press. ISBN 978-0-12-386455-0 (2014)

**Barrier properties to surrogates of hydrogenated carbon nano-films deposited on PET by plasma-enhanced chemical vapour deposition.**

E. C. Oliveira, Y. Echegoyen, C. Nerín, S. A. Cruz (GUIA)  
Food Additives and Contaminants Part A, 31, 1914-1927 (2014)

**Development of an active food packaging system with antioxidant properties based on green tea extract.**

D. Carrizo, G. Gullo, O. Bosetti, C. Nerín (GUIA)  
Food Additives & Contaminants: Part A, 31, 364-373 (2014)

**Diminution of Aflatoxin B1 production caused by an active packaging containing cinnamon essential oil.**

S. Manso, D. Pezo, R. Gómez-Lus, C. Nerín (GUIA)  
Food Control, 45, 101-108 (2014)

**Evaluation of two antimicrobial packaging films against Escherichia coli O157:H7 strains in vitro and during storage of a Spanish ripened sheep cheese (Zamorano).**

V. Otero, R. Becerril, J. Santos, J.M. Rodríguez-Calleja, C. Nerín, M.L. García-López (GUIA)  
Food Control, 42, 296-302 (2014)

**Migration of odorous compounds from adhesives used in market samples of food packaging materials by chromatography olfactometry and mass spectrometry (GC-O-MS).**

P. Vera, E. Canellas, C. Nerín (GUIA)  
Food Chemistry, 145, 237-244 (2014)

**Strategies to improve the solubility and stability of stilbene antioxidants: a comparative study between cyclodextrins and bile acids.**

F. Silva, A. Figueiras, E. Gallardo, C. Nerín, F. C. Domingues (GUIA)  
Food Chemistry, 145, 115-125 (2014)

**The additive properties of Oxygen Radical Absorbance Capacity (ORAC) assay: the case of essential oils.**

K. Bentayeb, P. Vera, C. Rubio, C. Nerin (GUIA)  
Food Chemistry, 148, 204-208 (2014)

**Molecular interactions between caffeine and catechins in green tea.**  
M. Colón, C. Nerín (GUIA)  
Journal of Agricultural and Food Chemistry, 62, 6777-6783 (2014)

**Migration of residual nonvolatile and Inorganic Compounds From Recycled post-consumer PET and HDPE.**  
C. Dutra, M.T.A. Freire, C. Nerín, K. Bentayeb, A. Rodriguez-Lafuente, M. Aznar, F.G.R. Reyes (GUIA)  
Journal of Brazilian Chemical Society, 25, 686-696 (2014)

**Atmospheric pressure gas chromatography coupled to quadrupole-time of flight mass spectrometry as a tool for identification of volatile migrants from autoadhesive labels used for direct food contact.**

E. Canellas, P. Vera, C. Nerín (GUIA)  
Journal of Mass Spectrometry, 49, 1181-1190 (2014)

**Three phases hollow fiber-liquid phase microextraction combined with HPLC-UV for determination of isothiazolinone biocides in adhesives used for food packaging materials.**

M. Rosero-Moreano, E. Canellas, C. Nerín (GUIA)  
Journal of Separation Science, 37, 272-280 (2014)

**Compounds from multilayer plastic bags cause reproductive failures in artificial insemination.**

C. Nerín, P. Alfaro, M. Aznar, E. Canellas, J. L. Ubeda, Y. Dahmani, C. Malo, R. Ausejo (GUIA)  
Nature Scientific Reports, 4, 4913 (2014)

**Anthropogenic lead emissions in the ocean – The evolving global experiment.**

E. Boyle, J. M. Lee, Y. Echegoyen, S. Moos, G. Carrasco, N. Zhao, J. Zhang, T. Gamo, H. Obata, K. Norisuye (GUIA)  
Oceanography, 27, 49-55 (2014)

**The recent distribution of lead in the Indian Ocean reflects the impact of regional emissions.**

Y. Echegoyen, J. M. Lee, E. A. Boyle, T. Gamo, H. Obata, K. Norisuye (GUIA)  
Proceedings of the National Academy of Sciences, 111, 15328-15331 (2014)

**Comparison of different extrusion processes for cleaning the recycled polypropylene removing volatile and non-volatile contaminants.**

P. S. Garcia, S. A. Cruz, C. Nerín (GUIA)  
Progress in Rubber, Plastics and Recycling Technology, 30, 37-54 (2014)

**Comparison between Solid Phase Microextraction (SPME) and Hollow Fiber Liquid Phase Microextraction (HFLPME) for determination of extractables from post-consumer recycled PET into food simulants.**

E. C. Oliveira, Y. Echegoyen, S. A. Cruz, C. Nerín (GUIA)  
Talanta, 127 59-67, (2014)

**Programa de simulación SIMLinks para cálculo de las consecuencias de accidentes en los que está involucradas sustancias peligrosas.**

C. Nerín, B. Seco, A. Tena, M. Calvo, G. Medina (GUIA)  
Actas del II Congreso Nacional de i+d en Defensa y Seguridad (DESEi+D). pp. 495-502. Dena Arto, A. et al. C. Univers. de la Defensa de Zaragoza. Zaragoza. ISBN: 978-84-940583-2-5 (2014)

**Programa de simulación SIMLinks para cálculo de las consecuencias de accidentes en los que está involucradas sustancias peligrosas.**

C. Nerín, B. Seco, A. Tena, M. Calvo, G. Medina (GUIA)  
Actas del II Congreso Nacional de i+d en Defensa y Seguridad (DESEi+D). pp. 495-502. Dena Arto, A. et al. C. Univers. de la Defensa de Zaragoza. Zaragoza. ISBN: 978-84-940583-2-5 (2014)

## **LABORATORIO DE ANÁLISIS DE AROMA Y ENOLOGÍA (LAAE)**

**Direct accurate analysis of cysteinylated and glutathionylated precursors of 4-mercaptop-4-methyl-2-pentanone and 3-mercaptophexan-1-ol in must by ultrahigh liquid chromatography coupled to mass spectrometry.**

B. Concejero, A. Peña-Gallego, P. Fernández-Zurbano, P. Hernández-Orte, V. Ferreira (LAAE)  
Analytica Chimica Acta, 812, 250-257 (2014)

**Chemical and sensory characterisation of the aroma of Çalkarası rosé wine.**

M. Darici, T. Cabaroglu, V. Ferreira, R. López (LAAE)  
Australian Journal of Grape and Wine Research, 20(3), 340-346 (2014)

**Characterization of lamb flavour from their aroma-active chemical composition in light lamb.**

M. Bueno, M.M. Campo, J. Cacho, V. Ferreira, A. Escudero (LAAE)  
Current Topics in Flavor Chemistry & Biology. Cap "Thermal flavor generation", pp. 350-353. Eds. T. Hofmann, D. Krautwurst and P. Schieberle. Deutsche Forschungsanstalt für Lebensmittelchemie. Germany. ISBN 978-3-938896-79-2 (2014)

**Changes in "key" wine aroma compounds during oxidation. Relationship with polyphenol changes and with some potential precursors.**

E. Franco, M. Bueno, L. Culleré, P. Fernández-Zurbano, V. Ferreira (LAAE)  
Current Topics in Flavor Chemistry & Biology. Cap "Chemistry and analysis of odorants, tastants and trigeminals", pp. 373-376. Eds. T. Hofmann, D. Krautwurst and P. Schieberle. Deutsche Forschungsanstalt für Lebensmittelchemie. Germany. ISBN 978-3-938896-79-2 (2014)

**Aroma compounds and sensory characteristics of Arneis Terre Alfieri DOC Wines: the concentration of polyfunctional thiols and their evolution in relation to different ageing conditions.**

F. Piano, M. Petrozziello, E. Vaudano, F. Bonello, V. Ferreira, J. Zapata, P. Hernández-Orte (LAAE)  
European Food Research and Technology, 239, 267-277 (2014)

**Gas chromatographic-olfactometric characterization of key aroma compounds in fresh and frozen lamb meat using new extraction methods.**

M. Bueno, V.C. Resconi, M.M. Campo, J. Cacho, V. Ferreira, A. Escudero (LAAE)  
Flavour Science, Part III: Flavor Systems, cap. 16, pp. 91-94. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Gas chromatography-olfactometric profiles of eight different varieties of Peruvian pisco spirits.**

L. Moncayo, L. Culleré, L., V. Ferreira, J. Cacho (LAAE)  
Flavour Science, Part III: Flavor Systems, cap. 42, pp. 221-226. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Importance of 3-Alkyl-2-Methoxypyrazines in Red Wines from Spain.**

E. Gracia, V. Ferreira, R. López (LAAE)  
Flavour Science, Part III: Flavor Systems, cap. 19, pp. 107-110. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**A robust SPME method for the analysis of wine volátiles based on multiple internal standards and multivariate regression.**

P. Herrero, J. Zapata, J. Cacho, V. Ferreira (LAAE)  
Flavour Science, Part IV: Instrumental Aspects and other Tools of the trade, cap. 86, pp. 465-469. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Automatic and Total Headspace In-Tube Extraction for the Accurate Determination of Polar Volatile Compound from Wines.**

J. Zapata, V. Ferreira, R. López (LAAE)

Flavour Science, Part IV: Instrumental Aspects and other Tools of the trade, cap. 76, pp. 407-409. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Evaluation of Gas Chromatography-Olfactometry for Screening Purposes of Wine Off-Flavors.**

A.de la Fuente, V. Ferreira, R. López (LAAE)

Flavour Science, Part IV: Instrumental Aspects and other Tools of the trade, cap. 79, pp. 423-428. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Problems in the analysis of VSCs and in the work with "oxygen-free" atmospheres.**

E. Franco, L. Culleré, D. Ruiz, A. Escudero, J. Cacho, V. Ferreira (LAAE)

Flavour Science, Part IV: Instrumental Aspects and other Tools of the trade, cap. 82, pp. 441-444. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Determination of volatile compounds for the assurance of quality, security and health in the use of alimentary oils and its application to home appliances.**

I. Ontañón, L. Culleré, V. Ferreira, A. Escudero (LAAE)

Flavour Science, Part VII: Practical and Industrial Aspects, cap. 151, pp. 627-630. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Evaluation of gamma and electron-beam irradiation on the aromatic profile of black truffles (*Tuber melanosporum*) and summer truffles (*Tuber aestivum*).**

L. Culleré, V. Ferreira, M.E. Venturini, P. Marco, D. Blanco (LAAE)

Flavour Science, Part VII: Practical and Industrial Aspects, cap. 101, pp. 553-556. Academic Press. Eds. V. Ferreira y R. López. ISBN 978-0-12-398549-1 (2014)

**Quantitative analysis of 3-alkyl-2-methoxypyrazines in German Sauvignon blanc wines by MDGC-MS or MDGC-MS/MS for viticultural and enological.**

C. Legrum, E. Gracia-Moreno, R. López, T. Potouridis, P. Slabizki, J. Weiand, H.G. Schmarr (LAAE)

European Food Research and Technology, 239, 549-558 (2014)

**Comparative analysis of aroma compounds and sensorial features of strawberry and lemon guavas (*Psidium cattleianum Sabine*).**

M.B. Egea, A.B. Pereira-Netto, J. Cacho, V. Ferreira, R. López (LAAE)

Food Chemistry, 164, 272-277 (2014)

**Extrinsic attributes responsible for red wine quality perception. A cross-cultural study between France and Spain.**

M.P. Sáenz-Navajas, J. Ballester, D. Peyron, D. Valentin (LAAE)

Food Quality and Preferences, 35, 70-85 (2014)

**Criteria to discriminate between wines aged in oak barrels and macerated with oak fragments.**

P. Hernández-Orte, E. Franco, C. González H., J. Martínez G., M. Cabellos, J. Suberviola, I. Orriols, J. Cacho (LAAE)

Food Research International, 57, 234-241 (2014)

**Sensory changes during bottle storage of spanish red wines under different initial oxygen doses.**

M.P. Sáenz-Navajas, J.M. Avizcuri, V. Ferreira, P. Fernández-Zurbano (LAAE)

Food Research International, 66, 235-246 (2014)

**Characterisation of the key odorants in a squid broth (*Illex argentinus*).**

V. Carrascón, A. Escudero, V. Ferreira, R. López G. (LAAE)

Food Science and Technology-LWT, 57(2), 656-662 (2014)

**Key changes in wine aroma active compounds during bottle storage of Spanish red wines under different oxygen levels.**

V. Ferreira, M. Bueno, E. Franco, L. Culleré, P. Fernández-Zurbano (LAAE)  
Journal of Agricultural and Food Chemistry, 62, 10015-10027 (2014)

**Quantitative analysis of free and bonded forms of Volatile Sulfur Compounds in wine. Basic methodologies and evidences showing the existence of reversible cation-complexed forms.**

E. Franco, V. Ferreira (LAAE)  
Journal of Chromatography A, 1359, 8–15 (2014)

**Simultaneous determination of free and bonded forms of odor-active carbonyls in wine using a headspace solid phase microextraction strategy.**

M. Bueno, J. Zapata, V. Ferreira (LAAE)  
Journal of Chromatography A, 1369, 33-42(2014)

**Influence of viticulture practices on grape aroma precursors and their relation with wine aroma.**

P. Hernández-Orte, B. Concejero Pardos, J. Astrain, B. Lacau, J. Cacho, V. Ferreira (LAAE)  
Journal of the Science of Food and Agriculture, 95(4), 688-701 (2014)

**A model explaining and predicting lamb flavour from the aroma-active chemical compounds released upon grilling light lamb loins.**

M. Bueno, M.M. Campo, J. Cacho, V. Ferreira, A. Escudero (LAAE)  
Meat Science, 98, 662-628 (2014)

**Wine, beer and cider: unraveling the aroma profile.**

A.Gamero, V. Ferreira, I.S. Pretorius, A. Querol (LAAE)  
Molecular Mechanisms in yeast carbon metabolism, cap. 10, pp. 261-297. Eds. J. Piskur, C. Compagno. Springer Berlin Heidelberg. ISBN 978-3-642-55012-6 (2014)

**LABORATORIO LÁSER Y MEDIO AMBIENTE (LASLAB)**

**Developing an environmental analysis of soils and water by spectrochemical techniques for undergraduate students of chemistry.**

J. Anzano, L. Abia, M. Aragonés, E. Ballano, B. Guzman, M.L. Lomero, C. Pena, E. Pérez (LASLAB)  
Journal of Laboratory Chemical Education, 2 (1), 4-9 (2014)

**Identification of Polymers by Means of LIBS.**

J. Anzano, C. Bello, R.H. Lasheras (LASLAB)  
Laser-Induced Breakdown Spectroscopy: Theory and Applications. Chapter 15, pp 1-18. Eds. S. Musazzi, U. Perini. Springer-Verlag Berlin. ISBN: 978-3-642-450 (2014)

**GRUPO DE INVESTIGACIÓN EN MÉTODOS DE ANÁLISIS RÁPIDOS (MARTE)**

**Progress in the determination of metalloids and non-metals by means of high-resolution continuum source atomic or molecular absorption spectrometry. A critical review.**

M. Resano, M.R. Flórez, E. García-Ruiz (MARTE)  
Analytical and Bioanalytical Chemistry, 406(9-10), 2239-2259 (2014)

**Potential of methyl fluoride as a universal reaction gas to overcome spectral interference in the determination of ultratrace concentrations of metals in biofluids using inductively coupled plasma-tandem mass spectrometry.**

E. Bolea-Fernández, L. Balcaen, M. Resano, F. Vanhaecke (MARTE)  
Analytical Chemistry, 86(15), 7969-7977 (2014)

**Accurate determination of ultra-trace levels of Ti in blood serum using ICP-MS/MS.**

L. Balcaen, E. Bolea-Fernández, M. Resano; F. Vanhaecke (MARTE)  
Analytica Chimica Acta, 809, 1-8 (2014)

**High-resolution continuum source graphite furnace atomic absorption spectrometry for direct analysis of solid samples and complex materials: a tutorial review.**

M. Resano, M.T. Aramendía, M.A. Belarra (MARTE)  
Journal of Analytical Atomic Spectrometry, 29(12), 2229-2250 (2014)