

## **PUBLICACIONES CIENTÍFICAS 2020**

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

#### **Size characterization and quantification of titanium dioxide nano- and microparticles-based products by Asymmetrical Flow Field-Flow Fractionation coupled to Dynamic Light Scattering and Inductively Coupled Plasma Mass Spectrometry.**

David Ojeda, M. Vanesa Taboada-López, Eduardo Bolea, Josefina Pérez-Arantegui, Pilar Bermejo-Barrera, Antonio Moreda-Piñeiro, Francisco Laborda (GEAS).  
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#### **Inorganic mass spectrometry.**

Josefina Pérez-Arantegui, Francisco Laborda (GEAS).  
Chemical Analysis in Cultural Heritage, chapter 3, pp 63-76. Eds. Luigia Sabbatini, Inez Dorothé van der Werf. Editorial De Gruyter. ISBN: 978-3-11-045648-6 (2020).

#### **Challenges in the data analysis of Asian lacquers from museum objects by pyrolysis gas chromatography/mass spectrometry.**

Diego Tamburini, Iliaria Bonaduce, Erika Ribechini, Erika, Carmen Gallego, Josefina Pérez-Arantegui (GEAS).  
Journal of Analytical and applied pyrolysis, 151, 104905 (2020).

#### **Colours of the "images of the floating world". Non-invasive analyses of Japanese ukiyo-e woodblock prints (18th and 19th centuries) and new contributions to the insight of oriental materials**

Carole Biron, Aurélie Mounier, Josefina Pérez-Arantegui, Gwénaëlle Le Bourdon, Laurent Servant, Rémy Chapoulie, Clodoaldo Roldán, David Almazán, Nerea Díez-De-Pinos, Floréal Daniel (GEAS).  
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#### **Voltammetric sensing of silver nanoparticles on electrodes modified with selective ligands by using covalent and electropolymerization procedures. Discrimination between silver(I) and metallic silver.**

Juan Carlos Vidal, Darío Torrero, Sonia Menés, Alvar de la Fuente, Juan R. Castillo (GEAS).  
Microchimica Acta, 187 (3), 183 (2020).

#### **About detectability and limits of detection in single particle inductively coupled plasma mass spectrometry.**

Francisco Laborda, Ana Cristina Gimenez-Ingalature, Eduardo Bolea, Juan R. Castillo (GEAS).  
Spectrochimica Acta Part B-Atomic Spectroscopy, 169, 105883 (2020).

#### **Cosmética y pigmentos de época romanorrepública en el Valle medio del Ebro: caracterización de muestras de La Cabañeta (El Burgo de Ebro, Zaragoza).**

José Antonio Mínguez Morales; Josefina Pérez-Arantegui (GEAS).  
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#### **Caracterización arqueométrica de la producción cerámica turolense a partir de mediados del siglo XIII.**

Antonio Hernández Pardos, Josefina Pérez-Arantegui (GEAS).  
Actas del XVII Congreso de la Asociación de Ceramología, Ojós/Murcia. Asociación de Ceramología, pp. 253-268. ISBN: 978-84-947289-2-1 (2020).

**Especiación de aditivos alimentarios metálicos en procesos digestivos in vitro: Detección de nanopartículas y formas disueltas.**

Celia Trujillo, Ana Crisrina Gimenez-Ingalaturre, Josefina Perez-Arantegui, Juan R. Castillo, Francisco Laborda (GEAS).  
Actualidad Analítica, 69, 25-28 (2020).

**Las mujeres de ciencias en la Universidad de Zaragoza.**

Carmen Magallón, Josefina Pérez-Arantegui (GEAS).  
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**GRUPO UNIVERSITARIO DE INVESTIGACIÓN ANALÍTICA (GUIA)**

**Influence of nonylphenol from multilayer plastic films on artificial insemination of sows.**

Cristina Nerín, Qi-Zhi Su, Paula Vera, Noelia Mendoza, Raquel Ausejo (GUIA).  
Analytical and Bioanalytical Chemistry, 412, 6519-6528 (2020).

**Direct Immersion - Solid-Phase Micro-extraction Coupled to Gas Chromatography - Mass Spectrometry and Response Surface Methodology for Non-target Screening of (Semi-) Volatile Migrants from Food Contact Materials.**

Qizhi Su, Paula Vera, Cristina Nerin (GUIA).  
Analytical Chemistry, 92, 7, 5577-5584 (2020).

**Impacts of food contact chemicals on human health: a consensus statement.**

Jane Muncke, Anna-Maria Andersson, Thomas Backhaus, Justin M. Boucher, Bethanie Carney Almroth, Arturo Castillo Castillo, Jonathan Chevrier, Barbara A. Demeneix, Jorge A. Emmanuel, Jean-Baptiste Fini, David Gee, Birgit Geueke, Ksenia Groh, Jerrold J. Heindel, Jane Houlihan, Christopher D. Kassotis, Carol F. Kwiatkowski, Lisa Y. Lefferts, Maricel V. Maffini, Olwenn V. Martin, John Peterson Myers, Angel Nadal, Cristina Nerin, Katherine E. Pelch, Seth Rojello Fernández, Robert M. Sargis, Ana M. Soto, Leonardo Trasande, Laura N. Vandenberg, Martin Wagner, Changqing Wu, R. Thomas Zoeller, Martin Scheringer (GUIA).  
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**Integration of untargeted and targeted mass spectrometry-based metabolomics provides novel insights into the potential toxicity associated to surfynol.**

Estefania Garcia-Calvo, Andres Machuca, Cristina Nerín, Noelia Rosales-Conrado, Daniela S. Anunciação, Jose L. Luque-Garcia (GUIA).  
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**Migration of volatile compounds from natural biomaterials and their safety evaluation as food contact materials.**

Esther Asensio, Laura Montañés, Cristina Nerín (GUIA).  
Food and Chemical Toxicology, 142, 111457 (2020).

**Migration of dihydroxyalkylamines from polypropylene coffee capsules to Tenax® and coffee by salt-assisted liquid-liquid extraction and liquid chromatography-mass spectrometry.**

Mahdiyeh Otoukesh, Paula Vera, Magdalena Wrona, Cristina Nerin, Zarrin Es'haghi (GUIA).  
Food Chemistry, 321, 126720 (2020).

**Migration studies and toxicity evaluation of cyclic polyesters oligomers from food packaging adhesives.**

Sara Ubeda, Margarita Aznar, Anna Kjerstine Rosenmai, Anne Marie Vinggaard, Cristina Nerín (GUIA).

Food Chemistry, 311, 125918 (2020).

**Comparison of two antioxidant packaging based on rosemary oleoresin and green tea extract coated on polyethylene terephthalate for extending the shelf life of minced pork meat.**

Xue-Chao Song, Elena Canellas, Magdalena Wrona, Raquel Becerril, Cristina Nerin (GUIA).  
Food Packaging and Shelf Life, 26, 100588 (2020).

**Discrimination of Virgin and Recycled Polyethylene Based on Volatile Organic Compounds Using a Headspace GC-MS Coupled with Chemometrics Approach.**

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**Graphene oxide/ Layered Double Hydroxides@ Sulfonated Polyaniline: a sorbent for ultrasonic assisted dispersive solid phase extraction of phthalates in distilled herbal beverages.**

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**Release of volatile compounds from cooking plastic bags under different heating sources.**

Margarita Aznar, Celia Domeño, Jazmin Osorio, Cristina Nerin (GUIA).

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**Bio-Based Materials for Active Food Packaging: Dream or Reality.**

Ângelo Luís, Fernanda C. Domingues, Filomena Silva (GUIA).

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**Ion mobility quadrupole time-of-flight high resolution mass spectrometry coupled to ultra-high pressure liquid chromatography for identification of non-intentionally added substances migrating from food cans.**

Elena Canellas, Paula Vera, Cristina Nerin, Nicola Dreolin, Jeff Goshawk (GUIA).

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**Ambient mass spectrometry as a tool for a rapid and simultaneous determination of migrants coming from a bamboo-based biopolymer packaging.**

Jazmín Osorio, Margarita Aznar, Cristina Nerín, Nicholas Birse, Christopher Elliott, Olivier Chevallier (GUIA).

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**Analytical Approaches for Analysis of Safety of Modern Food Packaging: A Review.**

Magdalena Wrona, Cristina Nerin (GUIA).

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**Encapsulation Systems for Antimicrobial Food Packaging Components: An Update.**

Raquel Becerril, Cristina Nerín, Filomena Silva (GUIA).

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**Phenolic compounds content and genetic diversity at population level across the natural distribution range of bearberry (*Arctostaphylos uva-ursi*, Ericaceae) in the Iberian peninsula.**

Esther Asensio, Daniel Vitales, Iván Pérez, Laia Peralba, Juan Viruel, Celia Montaner, Joan Vallès, Teresa Garnatje, Esther Sales (GUIA).

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**Characterization of odorants from baby bottles by headspace solid phase microextraction coupled to gas chromatography-olfactometry-mass spectrometry.**

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**Migration study of organotin compounds from food packaging by surface-enhanced Raman scattering.**

Luisa Mandrile, Martina Vona, Andrea Mario Giovannozzi, Jesús Salafranca, Gianmario Martra, Andrea Mario Rossi (GUIA).

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**Predicting the antioxidant capacity and total phenolic content of bearberry leaves by data fusion of UV-Vis spectroscopy and UHPLC/Q-TOF-MS.**

Xue-Chao Song, Elena Canellas, Esther Asensio, Cristina Nerin (GUIA).

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**Olive cake and leaf extracts as valuable sources of antioxidant and antimicrobial compounds: a comparative study.**

Messaad Moudache, Filomena Silva, Cristina Nerin, Farid Zaidi (GUIA).

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**Fourteen ethyl esters of wine can be replaced by simpler ester vectors without compromising quality but at the expense of increasing aroma concentration.**

Arancha de la Fuente Blanco, M. Pilar Sáenz-Navajas, Valentin, Dominique, Vicente Ferreira (LAAE).

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

**Sensory, olfactometric and chemical characterization of the aroma potential of Garnacha and Tempranillo winemaking grapes.**

Yohanna Alegre, M. Pilar Sáenz-Navajas, Purificación Hernández-Orte, Vicente Ferreira (LAAE).

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**Some clues about the changes in wine aroma composition associated to the maturation of "neutral" grapes".**

Ignacio Arias, Sara Ferrero Del Teso, M. Pilar Sáenz Navajas, Purificación Fernández Zurbano, Blanca Lacau, Jesús Astraín, Cristina Barón, Vicente Ferreira, Ana Escudero (LAAE).

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**Development of a new strategy for studying the aroma potential of winemaking grapes through the accelerated hydrolysis of phenolic and aromatic fractions (PAFs).**

Yohanna Alegre, Ignacio Arias, Purificación Hernández-Orte, Vicente Ferreira (LAAE).

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**Effect of aroma perception on taste and mouthfeel dimensions of red wines: Correlation of sensory and chemical measurements.**

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**Sensory variability associated with anthocyanic and tannic fractions isolated from red wines.**

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**Vineyard calcium sprays shift the volatile profile of young red wine produced by induced and spontaneous fermentation.**

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**Gas chromatography olfactometry (GC-O) for the (semi)quantitative screening of wine aroma.**

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**Investigating the Aroma of Syrah Wines from the Northern Rhone Valley Using Supercritical CO<sub>2</sub>-Dearomatized Wine as a Matrix for Reconstitution Studies.**

Olivier Geffroy, Marie Morère, Ricardo López, Grégory Pasquier, Jean S. Condoret (LAAE).  
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**Liquid chromatography-mass spectrometry-based metabolomics for understanding the compositional changes induced by oxidative or anoxic storage of red wines.**

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**Effect of grape maturity on wine sensory and chemical features: The case of Moristel wines.**

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**Revealing the usefulness of aroma networks to explain wine aroma properties: A case study of Portuguese wines.**

Silvia Petronilho, Ricardo López, Vicente Ferreira, Manuel A. Coimbra, Silvia M. Rocha (LAAE).  
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**NANOSENSORES Y SISTEMAS BIOANALITICOS (N&SB)**

**Smartphone-interrogated test supports for the enzymatic determination of putrescine and cadaverine in food.**

Isabel Sanz-Vicente, Angel López-Molinero, Susana de Marcos, Jesús Navarro, Pablo Cebrián, Chantal Arruego, Victor Visiedo, Javier Galbán (N&SB).  
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**Colorimetric-enzymatic determination of tyramine by generation of gold nanoparticles.**

Jesús Navarro, Susana de Marcos, Javier Galbán (N&SB).  
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**Analytical possibilities of Putrescine and Cadaverine enzymatic colorimetric determination in tuna based on diamine oxidase: A critical study of the use of ABTS.**

Jesús Navarro, Isabel Sanz-Vicente, Rebeca Lozano, Susana de Marcos, Javier Galbán (N&SB).  
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## **GRUPO DE INVESTIGACIÓN EN MÉTODOS DE ANÁLISIS RÁPIDOS (MARTE)**

**A simple and direct atomic absorption spectrometry method for the direct determination of Hg in dried blood spots and dried urine spots prepared using various microsampling devices.**

Flávio V. Nakadi, Raúl Garde, Marcia A.M.S. Da Veiga, Julio Cruces, Martín Resano (MARTE).  
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**Introducing multi-energy ratios as an alternative to multi-energy calibration for Br determination via high-resolution continuum source graphite furnace molecular absorption spectrometry. A case study.**

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**Understanding polyatomic interference in the determination of phosphorus via PO molecules using high-resolution continuum source graphite furnace molecular absorption spectrometry with direct solid analysis.**

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**Extraction induced by microemulsion breaking as a novel tool for the simultaneous determination of Cd, Mn, Pb and Sb in gasoline samples by ICP-MS and discrete sample introduction.**

Priscila O. Vicentino, Ricardo J. Cassella, Diego Leite, Martín Resano (MARTE).  
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**Breaking the boundaries in spectrometry. Molecular analysis with atomic spectrometric techniques.**

Martín Resano, M. Teresa Aramendía, Flávio V. Nakadi, Esperanza García-Ruiz, César Alvarez-Llamas, Nerea Bordel, Jorge Pisonero, Eduardo Bolea-Fernández, Tong Liu, Frank Vanhaecke (MARTE).  
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## **QUIMICA Y MEDIO AMBIENTE (QMA)**

**Local and remote sources of airborne suspended particulate matter in the antarctic region.**

César Marina, Luis V. Pérez-Arribas, Jesús Anzano, Jorge O. Cáceres (QMA).  
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**Direct determination of Al and Pb in waste printed circuit boards (PCB) by laser-induced breakdown spectroscopy (LIBS): Evaluation of calibration strategies and economic - environmental questions.**

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**Heavy metal transport and evolution of atmospheric aerosols in the Antarctic region.**

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**Quantitative analysis of major components of mineral particulate matter by calibration free laser-induced breakdown spectroscopy.**

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### **La Antártida, un paraíso para la investigación.**

Jesús Anzano, Jorge O. Cáceres, César Marina, L. Vicente Pérez-Arribas (QMA).  
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### **Química y Medio Ambiente.**

Jesús Anzano (QMA).  
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## **OTROS**

### **The intracellular number of magnetic nanoparticles modulates the apoptotic death pathway after magnetic hyperthermia treatment.**

Lilliane Beola, Laura Asín, Catarina Roma-Rodrigues, Yilian Fernandez-Afonso, Raluca M. Fratila, David Serantes, Sergiu Ruta, Roy W. Chantrell, Alexandra R. Fernandes, Pedro V. Baptista, Jesús Martínez de la Fuente, Valeria Grazu, Lucía Gutierrez.  
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### **The influence of cation incorporation and leaching in the properties of Mn-doped nanoparticles for biomedical applications.**

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### **New insights into the structural analysis of maghemite and (MFe<sub>2</sub>O<sub>4</sub>, M = Co, Zn) ferrite nanoparticles synthesized by a microwave-assisted polyol process.**

Álvaro Gallo-Cordova, Ana Espinosa, Aida Serrano, Lucía Gutiérrez, Nieves Menéndez, María Del Puerto Morales, Eva Mazarió.  
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### **Smartphone-Based Colorimetric Method to Quantify Iron Concentration and to Determine the Nanoparticle Size from Suspensions of Magnetic Nanoparticles.**

Yilian Fernández-Afonso, Gorka Salas, Irene Fernández-Barahona, Fernando Herranz, Cordula Grüttner, Jesús Martínez de la Fuente, María del Puerto Morales, Lucía Gutiérrez.  
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