13as JORNADAS DE ANÁLISIS INSTRUMENTAL

RECINTO GRAN VIA. 14-16 NOVIEMBRE 2011

EXPOQUIMIA
Salón Internacional de la Química

Fira Barcelona

Año Internacional de la QUÍMICA 2011

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Sociedad Española de Química Analítica

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PROGRAMA CIENTÍFICO

La Sociedad Española de Química Analítica (SEQA) organiza el programa científico de las jornadas en colaboración con la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA), la Sociedad de Espectroscopia Aplicada (SEA), la Sociedad Española de Espectrometría de Masas (SEEM) y la Sociedad Española de Proteómica (SEProt).

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OC =	ORAL CORTA P = PÓSTER
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Día 14 de Noviembre de 2011 (Lunes)

Hora	Sala 4.1	Sala 4.2
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9.00-9.30	**Ceremonia de apertura:** Mesa: Dra. Elena Domínguez y Dr. Joan O. Grimalt	
9.30-10.30	**CONFERENCIA PLENARIA: Prof. R. Graham Cooks** ***Miniature mass spectrometers and ambient ionization: Instrumentation and applications in tissue imaging, disease diagnostics, food & public safety"*** Mesa: Dra. Elena Domínguez y Dra. María Teresa Galcerán	
10.30-11.00	Colocación de posters **(TODOS LOS TEMAS)** CAFÉ	
11.00-11.30	**Conferencia invitada: Prof. Joan Albaigés** ***"The characterization of oil spills: a challenge for analytical chemistry"*** Mesa: Dra. Carmen Cámara	
11.30-13.00	**Comunicaciones MAMOC01A a MAMOC07** Mesa: Dra. Lourdes Cantón y Dr. Luis F. Capitán	**Comunicaciones AYMOC01 a AYMOC03** **NANOC01 a NANOC04** Mesa: Dr. Miguel Valcárcel y Dr. Antonio Molina
13.00-14.00	**COMIDA**	
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15.00-16.00	**CONFERENCIA PLENARIA: Prof. Luis M. Liz-Marzan** **"Ultrasensitive analysis using metal nanoparticles"** Mesa: Dr. Xavier Ríus	
16.00-16.30	**Conferencia invitada: Dra. Francisca Mulero** **"PET-CT in preclinical cancer research** Mesa: Dr. J.M. Vadillo	
16.30-17.30	**Comunicaciones MAMOC08 a MAMOC12** Mesa: Dr. Manuel Hernández y Dr. J. Luis Pérez Pavón	**Comunicaciones DIAOC01 a DIAOC05** Mesa: Dr. Víctor Cerdá y Dr. Arsenio Muñoz de la Peña
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18.00-19.00	**Discusión de Posters** **MAMP01 a MAMP82** Mesa: Dra. Carmen Cámara y Dra. Elena Ibáñez	**Discusión de Posters** **AYMP01 a AYMP13** **NANPO1 a NANP10** **DIAP01 a DIAP21** Mesa: Dra. Soledad Muniategui y Dr. Arsenio Muñoz de la Peña **ASAMBLEA SEA (sala 4.3)**

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Hora	Sala 4.1	Sala 4.2
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10.00-10.30	**Conferencia invitada: Profª. Cristina Nerín** ***Influence of packaging on food safety: Analytical challenges"*** Mesa: Dr. Esteban Abad	
10.30-11.00	CAFÉ	
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12.00-13.00	**Comunicaciones CSAOC06 a CSAOC10** Mesa: Dr. Damiá Barceló y Dr. Rafael Cela	Sesión: **ETBs-CDTI-EMPRESAS** Coordinadores: Dra. Arantxa Narváez Dra. Rosa Puchades Dr. Tolo Simonet
13.00-14.00	COMIDA	
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14.00-15.00	Visita posters Calidad y seguridad alimentaria, Biosensores, Electroquímica, Análisis Clínicos, Análisis de Productos farmacéuticos y Especiación	ASAMBLEA DEL GRUPO DE ESPECIACIÓN DE LA SEQA
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15.00-16.00	**CONFERENCIA PLENARIA: Profª. Jenny Emnéus** ***"Exploring cellular dynamics at nanoscale"*** Mesa: Dr. J. M. Vadillo	
16.00-17.30	**SEQA: Sesión de docencia** Mesa: Dr. Manuel Hernández-Dra. Encarna Lorenzo- Dr. Luis F. Capitan	**Sesión jóvenes Investigadores** Coordinador: Dr. José Luis Luque
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	CENA DE LA REUNIÓN	

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10.00-11.00	**CONFERENCIA PLENARIA: Prof. Pier Giorgio Righetti** ***The proteome Argonauts: conquering the "golden fleece" of alcoholic beverages and soft drinks via combinatorial peptide ligands*** Mesa: Dr. Joan O. Grimalt y Dra. M. José González Carlos	
11.00-11.30	CAFÉ	
11.30-12.00	**Conferencia invitada: Dr. Manuel Fuentes García** **"Protein chips in biomarker & drug discovery"** Mesa: Dr. Alfredo Sanz-Medel	
12.00-13.00	**Comunicaciones PRTOC01 a PRTOC02** **Comunicaciones OAIOC01 a OAIOC03** **Comunicación APIOC01** Mesa: Dr. Fernando J. Corrales y Dr. Javier Santos	**JORNADAS TÉCNICAS** **Coordinadores:** Dr. José Luis Pérez Pavón y Dra. Soledad Muniategui
13.00-14.00	COMIDA	
14.00-15.00	Visita posters Contribuciones Teóricas y Quimiometría, Docencia, Proteómica, Otros Campos del Análisis Instrumental, Análisis de procesos y productos industriales	
15.00-15.30	**Conferencia invitada: Prof. Jordi Segura Noguera** ***"Antidoping control, cross road between Chemistry and other Life Sciences"*** Mesa: Dr. Enrique Barrado	
15.30-16.30	**Discusión de poster CSAP01 A CSAP85** Mesa: Dr. Juan Cacho, Dr. Jesús Hernández, Dr. Javier Santos	**Discusión de poster AClP01 a AClP10; APFP01 a APF13; BIOP01 a BIOP011; ELCP01 A ELCP04; APIP01 a API05** Mesa: Dra. Rosa Puchades, Dr. Santiago Maspoch
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SESIONES CIENTÍFICAS – LUNES 14 DE NOVIEMBRE

08:30 **Recogida de documentación**

09:00 **Ceremonia de Apertura (*Sala 4.1*)**
Mesa: Dra. Elena Domínguez y Dr. Joan O. Grimalt

09:30 **Conferencia Plenaria** (*Sala 4.1*) – **Moderadoras:** Dra. Elena Domínguez y Dra. Mª Teresa Galceran
Prof. R. Graham Cooks
"Miniature mass spectrometers and ambient ionization: Instrumentation and applications in tissue imaging, disease diagnostics, food & public safety"

10:30 **Colocación de Posters (TODOS LOS TEMAS) / Café**

11:00 **Conferencia invitada** (*Sala 4.1*) – **Moderadora:** Dra. Carmen Cámara
Dr. Joan Albaigés
"The characterization of oil spills: A challenge for analytical chemistry"

11:30 **Comunicaciones Orales**: Medio Ambiente **(*Sala 4.1*)**
Moderadores: Dra. Lourdes Cantón y Dr. Luis F. Capitán

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OC02 E. Barón González ; I. Rudolph ; R. Barra ; E. Eljarrat ; D. Barceló

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OC04 R. Bouza Deaño ; M. López Sepúlveda ; J.C. Mohino Guerrero

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MAM-OC05 N. Fontanals Torroja ; R.M. Marcé ; F. Borrull

ON-LINE SOLID-PHASE EXTRACTION COUPLE TO LIQUID CHROMATOGRAPHY – MASS SPECTROMETRY

OC06 H. Gallart Ayala ; C.P.B. Martins ; M. Soto ; E. Moyano ; M.T. Galceran ; J. Caixach

RECENT DEVELOPMENTS IN THE ANALYSIS OF GLYPHOSATE AND AMPA IN WATER SAMPLES BY LC-MS/MS AND HRMS

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Moderadores: Dr. Miguel Valcárcel y Dr. Antonio Molina

AYM-OC01 M.M. Barrios Romero ; A. González Crevillén ; J.C. Diez-Masa

APPLICATION OF SU-8 MICROFLUIDIC DEVICES TO WHEY PROTEIN ANALYSIS

M. Miró

AUTOMATED SAMPLE PREPARATION IN ENVIRONMENTAL AND BIOANALYTICAL ASSAYS USING MESO/MICROFLUIDIC PLATFORMS

I.M. Pedron Ruiz ; J.G. March ; J.L. Benedé ; A. Salvador ; A. Chisvert

A NEW THREE-PHASE MEMBRANE-ASSISTED LIQUID-PHASE MICROEXTRACTION METHOD: DETERMINATION OF NITRITE IN TAP WATER SAMPLES AS MODEL ANALYTICAL APPLICATION

NAN-OC01 J.M. Abad Pastor ; A.Y. Tesio ; J.L. Pau ; F. Pariente ; J. Piqueras ; E. Lorenzo

METALLIC NANOELECTRODES FABRICATION FOR THE DEVELOPMENT OF NANOSTRUCTURED PLATFORMS BY SCANNING ELECTROCHEMICAL MICROSCOPY (SECM)

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T. Díaz-Faes ; M.E. Díaz García ; M.J.A. García Calzón ; R. Badía Laíño

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13:00 **Comida**

14:00 **Visita Posters**: Medio Ambiente. Automatización y Miniaturización. Nanotecnología. Desarrollos en Instrumentación Analítica

15:00 **Conferencia Plenaria** (*Sala 4.1*) – **Moderador:** Dr. Xavier Ríus
Prof. Luis M. Liz-Marzán
"Ultrasensitive analysis using metal nanoparticles"

16:00 **Conferencia invitada** (*Sala 4.1*) – **Moderador:** Dr. J.M. Vadillo
Dra. Francisca Mulero
"PET-CT in preclinical cancer research"

16:30 **Comunicaciones Orales**: Medio Ambiente **(*Sala 4.1*)**
Moderadores: Dr. Manuel Hernández y Dr. J. Luis Pérez Pavón

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Moderadores: Dr. Víctor Cerdá y Dr. Arsenio Muñoz de la Peña

DIA-OC01 M. Ariza Avidad ; N. López Ruiz ; A. Martínez Olmos ; J. Vukovic ; J. Banqueri ; L.F. Capitan

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DIA-OC03

DIA-OC04

DIA-OC05

17:00 **Pausa / Café**

18:00 **Discusión de Posters**: Medio Ambiente**. (*Sala 4.1*)**
Moderadoras: Dra. Carmen Cámara y Dra. Elena Ibáñez

18:00 **Discusión de Posters**: Automatización y Miniaturización. Nanotecnología. Desarrollos en Instrumentación Analítica. **(*Sala 4.2*)**
Moderadores: Dra. Soledad Muniategui y Dr. Arsenio Muñoz de la Peña

18:00 **Asamblea SEA**. **(*Sala 4.3*)**

SESIONES CIENTÍFICAS – MARTES 15 DE NOVIEMBRE

09:00 **Conferencia Plenaria** (*Sala 4.1*) – **Moderadores:** Dr. J.M. Pingarrón y Dra. Encarnación Lorenzo
Sesión "in Memoriam" del *Prof. Lucas Hernández*
Prof. Richards M. Crooks
"Bipolar electrodes: fundamentals, sensing, and concentration enrichment in microelectrochemical systems"

10:00 **Conferencia invitada** (*Sala 4.1*) – **Moderador:** Dr. Esteban Abad
Profª. Cristina Nerín
"Influence of packaging on food safety: Analytical challenges"

10:30 **Café**

11:00 **Comunicaciones Orales**: Calidad y Seguridad Alimentaria **(*Sala 5.1*)**
Moderadores: Dr. Juan Cacho y Dr. Jesús Hernández

CSA-OC02

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CSA-OC04

CSA-OC05 C. Nerin ; E. Canellas ; P. Alfaro ; C. Domeño

IDENTIFICATION OF NON INTENTIONALLY ADDED SUBSTANCES (NIAS) IN NEW ACTIVE FOOD PACKAGING PROTOTYPES

11:00 **Comunicaciones Orales**: Biosensores. Electroquímica **(*Sala 5.2*)**
Moderadoras: Dra. Elena Domínguez y Dra. Encarnación Lorenzo

BIO-OC01 S. Liébana ; D. Spricigo ; M.P. Cortés ; M. Llagostera ; S. Alegret ; M.I. Pividori

BIO-OC02

BIO-OC03

BIO-OC04

ELC-OC01

12:00 **Comunicaciones Orales**: Calidad y Seguridad Alimentaria **(*Sala 5.1*)**
Moderadores: Dr. Damiá Barceló y Dr. Rafael Cela
CSA-OC06

ANALYSIS OF FULLERENES (C60 TO C84) AND C60-FULLERENE DERIVATIVES BY LC-APPI-MS

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P. Rodríguez González ; A. González Antuña ; M. Fernández Fernández ; J.I. García Alonso

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N. Unceta ; Z. Abrego ; M. Montaña ; L. Echeazarra ; J. Sallés ; R.J. Barrio

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J.A. Zapata Ochoa ; J. Cacho ; V. Ferreira

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12:00 **Sesión. ETBs-CDTI-EMPRESAS. (*Sala 5.2*)**
Coordinadores: Dra. Arantxa Narváez; Dra. Rosa Puchades y Dr. Tolo Simonet

13:00 **Comida**

14:00 **Visita Posters**: Calidad y seguridad alimentaria. Biosensores. Electroquímica. Análisis Clínicos. Análisis de Productos farmacéuticos. Especiación.

15:00 **Conferencia Plenaria (*Sala 4.1*)** – **Moderador:** Dr. J.M. Vadillo
Prof[a]. Jenny Emnéus
"Exploring cellular dynamics at nanoscale"

16:00 **Sesión de Docencia. SEQA. (*Sala 4.1*)**
Moderadores: Dr. Manuel Hernández; Dra. Encarna Lorenzo y Dr. Luis F. Capitan

16:00 **Sesión. Jóvenes investigadores**. **(*Sala 4.2*)**
Coordinador: Dr. José Luis Luque

17:30 **Pausa / Café**

18:00 **Asamblea SEQA**. **(*Sala 4.1*)** 18:00 **Asamblea SECYTA**. **(*Sala 4.2*)**

CENA DE LA REUNIÓN

SESIONES CIENTÍFICAS – MIERCOLES 16 DE NOVIEMBRE

09:00 **Comunicaciones Orales**: Análisis Clínico. Análisis de productos farmacéuticos. **(*Sala 4.1*)**
Moderadoras: Dra. Yolanda Picó y Dra. Mª Teresa Galceran

ACl-OC01

ACl-OC02

APF-OC01

APF-OC02

APF-OC03

09:00 **Comunicaciones Orales**: Especiación. Contribuciones Teóricas y Quimiometría. (*Sala 4.2*)
Moderadores: Dr. Marcelo Blanco y Dr. Santiago Maspoch

ESP-OC01

ESP-OC02

ESP-OC03

CTQ-OC01

CTQ-OC02

10:00 **Conferencia Plenaria (*Sala 4.1*)** – **Moderadores:** Dr. Joan O. Grimalt y Dra. M. José González
Prof. Pier Giorgio Righetti
"The proteome Argonauts: conquering the "golden fleece" of alcoholic beverages and soft drinks via combinatorial peptide ligands"

11:00 **Pausa / Café**

11:30 **Conferencia invitada (*Sala 4.1*)** – **Moderador:** Dr. Alfredo Sanz-Medel
Dr. Manuel Fuentes García
"Protein chips in biomarker & drug discovery"

12:00 **Comunicaciones Orales**: Proteómica. Otros campos del Análisis instrumental. Análisis de Procesos y Productos Industriales. (*Sala 4.1*)
Moderadores: Dr. Fernando J. Corrales y Dr. Javier Santos
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PRT-OC02

OAI-OC01

OAI-OC02

OAI-OC03 ;

API-OC01

12:00 **JORNADAS TÉCNICAS** (*Sala 4.2*)
Coordinadores: Dr. José Luis Pérez Pavón y Dra. Soledad Muniategui

13:00 **Comida**.

14:00 **Visita Posters**: Contribuciones Teóricas y Quimiometría. Docencia. Proteómica. Otros Campos del Análisis Instrumental. Análisis de Procesos y Productos Industriales.

15:00 **Conferencia invitada** (*Sala 4.1*) – **Moderador:** Dr. Enrique Barrado
Prof. Jordi Segura Noguera
"Antidoping control, cross road between Chemistry and other Life Sciences"

15:30 **Discusión de Posters**. Calidad y Seguridad Alimentaria. **(*Sala 4.1*)**
Moderadores: Dr. Juan Cacho, Dr. Jesús Hernández y Dr. Javier Santos

15:30 **Discusión de Posters**. Análisis Clínico. Análisis de productos farmacéuticos. Biosensores. Electroquímica. Análisis de Procesos y Productos Industriales. **(*Sala 4.2*)**
Moderadores: Dra. Rosa Puchades y Dr. Santiago Maspoch

16.30 **Discusión de Posters.** Contribuciones teóricas y Quimiometría, Proteómica, Especiación, Otros Campos AI, Análisis de Procesos y Productos industriales **(*Sala 4.2*)**
Moderadores: Dr. Alfredo Sanz Medel y Dr. Enrique Barrado

17:30 **Ceremonia de clausura**.

Mesa: Dra. Elena Domínguez y Dr. Joan O. Grimalt
Entrega de Premios. Cóctel de despedida.

CONFERENCIA PLENARIA

Miniature mass spectrometers and ambient ionization: instrumentation and applications in tissue imaging, disease diagnostics, food & public safety

R. Graham Cooks
Department of Chemistry & Center for Analytical Instrumentation Development, Purdue University, West Lafayette, IN 47907

(Henry B. Hass Distinguished Professor—Analytical Chemistry)
http://www.chem.purdue.edu/people/faculty/faculty.asp?itemID=1)

The recent development of ambient ionization methods is transforming the applications of mass spectrometry allowing virtually any sample to be examined in air, rather than being introduced into the mass spectrometer vacuum system. Ambient ionization methods include the spray method, desorption electrospray ionization (DESI) in which the sample is impacted by charged microdroplets which pick up analyte by dissolution and carry it to the MS; plasma-based methods among them low temperature plasma (LTP) and the new paper spray (PS) ionization method. The physical and mechanistic basis of each of these experiments will be described.

DESI finds application in disease diagnosis by tissue imaging and examples of human bladder, liver and brain cancer diagnostics will be given. In another application, whole blood analysis for therapeutics is achieved in a few seconds using another new method, paper spray. LTP applications in food safety and bacterial identification will be described.

Other examples of applications include transportation security, forensic applications and cleaning validation as well as natural products characterization.

The talk will conclude with information on the combination of ambient ionization methods with handheld miniature mass spectrometers, a tool that has great potential for the discovery chemist as well as in practical applications in industry and medicine.

CONFERENCIA PLENARIA

Ultrasensitive Analysis Using Metal Nanoparticles

Luis M. Liz-Marzán

Departamento de Química Física and Unidad Asociada CSIC-Universidade de Vigo, 36310 Vigo, Spain, lmarzan@uvigo.es.

http://webs.uvigo.es/coloides/nano/

Metal nanoparticles display very interesting optical properties, related to localized surface plasmon resonances (LSPR), which give rise to well-defined absorption and scattering peaks in the visible and near-IR spectral range. Such resonances can be tuned through the size and shape of the nanoparticles, but are also extremely sensitive towards dielectric changes in the near proximity of the particles surface. Therefore, metal nanoparticles have been proposed as ideal candidates for biosensing applications, on the basis of concepts similar to those applied in commercial SPR biosensors. Additionally, localized surface plasmon resonances are characterized by large electric fields at the surface, which are responsible for the so-called surface enhanced spectroscopies, and in particular for surface enhanced Raman scattering (SERS). Since the Raman scattering cross sections can be enhanced up to 12 orders of magnitude, very small amounts of analyte can be detected and thus the SERS effect has rendered Raman scattering spectroscopy a powerful analytical technique that allows ultrasensitive chemical or biochemical analysis. However, practical application of SERS is hindered by problems related to optimization and reproducibility of the enhancement factors, uniformity of the substrates and proximity of the analyte molecules to the metallic surface. In this communication, we present several examples of novel strategies based on colloid chemistry, to fabricate highly efficient nanostructured SERS substrates that overcome some of the drawbacks of the technique. Shape control, directed nanoparticle assembly, and different types of responsive polymer substrates have been shown to yield ultrasensitive detection of a wide variety of analytes, including environmental contaminants such as dioxins or DDT, as well as infectious proteins such as scrambled prions.

References:

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CONFERENCIA PLENARIA

Bipolar electrodes: fundamentals, sensing, and concentration enrichment in microelectrochemical systems

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This presentation focuses on the fundamental principles of bipolar electrochemisty and how systems based on these principles can be used for chemical sensing and concentration enrichment of analytes present at low concentration. An important aspect of bipolar electrodes (BPEs) is that they do not require a direct external electrical connection, and this means they are well-suited for both nanoscale electrochemistry applications, where it might be difficult to make such connections, and for high-density electrode arrays, where it would be impractical to make thousands or millions of individual electrode connections.

The talk will begin with a comparison of traditional three-electrode electrochemisty and bipolar electrochemistry. The key point here is that both methods rely on exerting control over the potential difference at the electrode/solution interface, but in bipolar electrochemisty it is the potential of the solution that is modulated rather than the electrode potential. Another important aspect of bipolar electrochemistry is that the rates of faradaic processes at the anodic and cathodic poles of a BPE must be identical to ensure charge neutrality. Accordingly, it is possible to use an observable electrochemical process, such as silver electrodissolution, as an indirect measure of the current associated with a sensing event at the cathodic pole of the BPE. Because silver dissolution can be observed visually, it is possible to simply and simultaneously read-out electrochemical array sensors consisting of thousands of electrodes.

Bipolar electrodes can also be configured to modulate the local electric field within a microfluidic channel. This means it is possible to balance the electroosmotic and electrophoretic velocity of an analyte at a particular location in a channel. We will discuss the fundamental principles of this process in the context of both high-level simulations and experiments, and then demonstrate an application that leads to analyte concentration enrichment by a factor of 500 000, and a second application in which the BPE enables simultaneous enrichment and separation. BPEs can also be used to bring two separated microfluidic channels into electrical contact, and this provides a means for implementing a method we call faradaic ion concentration polarization.

CONFERENCIA PLENARIA

Exploring Cellular Dynamics at Nanoscale

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"Exploring Cellular Dynamics at Nanoscale" (EXCELL) is a multidisciplinary EU FP7 collaboration to design novel Lab-on-a-Chip tools required for real-time monitoring of cellular dynamics not usually employed in Biology. This lecture presents course of developments towards a microfluidic array cell culture and analysis system. The compactness of the system facilitates monitoring of cellular dynamics using an integrated electrode microchip comprising 12 electrode arrays and ports for optical detection and an ad-hoc low noise multichannel potentiostat to obtain an optimal signal to noise ratio for precise measurements from single cells or a small cell population. The designed and fabricated 24-channel potentiostat facilitates different electrochemical techniques, such as low noise amperometric recordings down to low pA level, fast scan cyclic voltammetry (CV) up to 2.5 kV/s and fast impedance spectroscopic (IS) tracking from 1 mHz to 100 kHz. All the electrochemical assays and analysis of the recorded results are conducted using a custom-made software. Microfluidic experiments are run using a programmable multichannel pump platform, which is operated by step motor-driven peristaltic micropumps. The culture system with integrated electrode microchip is mounted on the pump platform and coupled to the potentiostat to form a complete Lab-on-a-Chip experimental setup. The programmability allows fluidic delivery in complex patterns making possible to run on-line electrode cleaning, modification, cell seeding, culturing, and cell-based analytical assays. The design of the cell culture chambers was shown to be suitable for cell seeding, perfusion culture and performing electrochemical assays. The usability of the presented system is demonstrated with two cell-based applications: monitoring of (i) redox metabolism and seeding of yeast cells and (ii) dopamine exocytosis from cultivated PC12 cells. Validation of results from yeast cells and a population of PC12 cells will be largely discussed.

CONFERENCIA PLENARIA

The proteome Argonauts: conquering the “golden fleece” of alcoholic beverages and soft drinks via combinatorial peptide ligands

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Proteomic science has been vastly exploited in the past ten years for biomarker discovery in sera, in search of panels of proteins able to warn about the onset of various diseases. According to Mitchell (Nature Biotech. 28, 2010, 665-670), this has been the biggest “fiasco” in this arena, with billions of dollars wasted. Completely different results have been obtained by us when analyzing a “fiasco” (a 1.5 liter jug) of white or red wine, with the combinatorial peptide ligand library (CPLL) technology. It turns out that most wine producers treat white wines with casein (and red wines with egg albumen) in order to eliminate residual grape proteins that would flocculate upon long term storage. Although required by EC rulers, no producer has ever stated the residual amount of these allergenic additives in their product. With the CPLL technology, we were able to detect as little as 1 µg casein/L, an extremely high detection sensitivity, unreported up to the present (the official ELISA test of the EC reached barely down to 200 µg/L). However, if untreated wines are analyzed, we can detect well over 100 residual grape proteins present in wines, this suggesting the possibility of proteo-typing grand crus against counterfeited products invading the market. We will additionally report proteo-typing of beers as well as different carbonated soft beverages. One could thus easily distinguish among artificial beverages, made only with synthetic additives and flavours (Coca Cola being a classical example) vs. genuine products made with plant extracts. Examples will be given on proteome analysis of, e.g., almond milk, orgeat, Cola beverages and the like. Regulatory agencies and customers would thus have a new, formidable tool for protection against adulterated and counterfeited foodstuff and beverages.

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COMUNICACIÓN INVITADA

THE CHARACTERIZATION OF OIL SPILLS: A CHALLENGE FOR ANALYTICAL CHEMISTRY

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Marine pollution by oil is a well known problem that has become particularly evident at the time of massive accidental spills, such as the *Prestige* or, more recently, the *Deepwater Horizon* platform in the Gulf of Mexico. However, operational discharges in coastal areas or offshore (e.g. urban effluents or oil tank washings) are more widespread and become confused with the accidental spills, when the acute phase is gone.

To illustrate the relevance of the problem, Figure 1 shows the number of spills detected by satellite to over 2009 in European coastal waters.

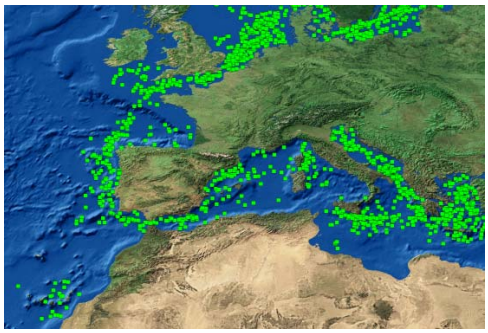

Figure 1. Remote sensing of oil spills in 2009
(European Maritime Safety Agency / CleanSeaNet 2010)

In order to address the issues that such discharges pose, including their early detection and the precise determination of the sources, in the last decade significant advances have been taking place thanks to the contributions, among others, of the Instrumental Analysis.

The presentation will show the approach taken in Europe to establish a surveillance system of oil spills, from remote sensing to the collection of samples and their final identification. Efficient and unambiguous analytical methods for the characterization of these spillages are needed from the standpoint of the enforcement of the pollution control laws, designed to protect the public health and the environment. In this respect, we will describe the methodology adopted and currently assessed by the *Oil Spill Identification Network of Experts* (OSINET), which will be illustrated by the results of several real cases.

Sampling is the first step in obtaining information about the spill. Designing a comprehensive oil source sampling plan is fundamental in the investigative efforts of an oil spill, and collection of oil

from both the spill and the suspected source(s) is crucial to any forensic program. Sampling at sea is carried out with special devices for collecting surface oil, patches, slicks or sheens. Sampling of tanks on the vessels must be comprehensive and representative. The chain of custody of the samples is essential to ensure the validity of any disciplinary process that may arise.

The identification of the samples is carried out by GC-MS, considering different sectors of the chromatographic profile and the hydrocarbon families associated with them. These include *n*-alkanes, acyclic isoprenoids, sesquiterpanes, steranes, triterpanes and alkyl aromatics. To this end, a number of source and weathering indices, based on the determination of specific compounds (molecular markers) have been proposed for comparison of samples, and multivariate statistical methods are applied to improve the diagnostic capability of this methodology. Obviously, the specific distributions of hydrocarbon families need to be properly used for the characterization of the spills. Particularly, the effects of the processes of evaporation, dissolution, photooxidation and biodegradation on the spilled samples need to be taken into account for the adequate interpretation of the results.

The samples are considered to match to a high degree of scientific certainty when the differences in the chromatographic patterns and diagnostic ratios of samples submitted for comparison are lower than the variability of the method or can be explained unequivocally, for example by weathering. These criteria are illustrated with examples of accidental and operational discharges.

Among the former we refer to a spill of heavy fuel oil following the *Tricolor* and *Vicky* incident in the British Channel, and another in the Strait of Gibraltar (Figure 2). In both cases, the aging of the samples collected at sea was a factor to be taken into account when making comparisons with reference samples. The diagnostic criteria used in the comparison of potential sources with different samples collected at sea, showing varying degrees of evaporation and photooxidation will be shown.

Figure 2. Oil spill in the Strait of Gibraltar (Source: SASEMAR)

Among the operational discharges, the most common are those related to washing tanks or bilges. In this case, the identification of such residues is particularly difficult because its composition, a mixture of products used in a vessel (fuel oils and lubricating oils), is very variable. The lack of homogeneity of the samples stored in the bilge is the main difficulty. The difficulties are even more important when spills occur in ports, where potential sources are numerous. In this case, we present two cases of spills occurred in fishing ports, where the cause of the spill among four potential sources should be identified.

COMUNICACIÓN INVITADA

"PET-CT in preclinical cancer research"

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http://www.cnio.es/es/index.asp

In the field of molecular imaging, in-vivo preclinical imaging has become increasingly important to academic researchers and especially to those involved in the drug development process. Recent improvements in the Molecular Imaging technologies employed to image small animals are helping to generate better data, and at a more prodigious rate than ever.

In the past, mouse & rat models of Human Disease are usually studied using invasive techniques, which sacrifice the animal. Although these techniques are well established, there are several major disadvantages to this approach:

- A large number of animals is necessary in order for a study to achieve statistical significance
- Follow-up or longitudinal studies are generally not possible on the same animal
- Metabolism studies, for efficacy, are difficult to obtain
- A large amount of economic and labor resources is required

However, over the past few years, in vivo Imaging Systems for small animals have become increasingly popular, including:

- X-ray micro CT (computed tomography)
- MRI (magnetic resonance imaging)
- Ultrasound
- Micro-PET (positron emission tomography)
- Micro-SPECT (single photon emission computed tomography)
- Optical (luminescence & fluorescence)

Of these technologies, only the Nuclear Imaging Modalities (PET & SPECT) can provide the sensitivities required to obtain the same physiological imaging acuity in small animals as can be obtained from humans. These modalities greatly facilitate the translation of preclinical studies to applications in the clinic!

Micro-PET-CT (Multimodality):

- Best suited for small molecules and molecules with fast assay kinetics
- Higher sensitivity (3-4% on average)
- Strong quantitation
- Sensitivity and resolution nonuniform throughout imaging chamber
- Expensive tracers with short half-lives, lower specific activity
- Subject receives 5-10x radiation dose of SPECT

Tumour imaging in live mice has opened new avenues for research and the ability to perform longitudinal studies in combination with therapeutic interventions using a wide range of techniques.

In our group we have developed methods to optimise visualisation of murine tumours using 18F-FDG, F18-MISO, Gallium 68 etc PET, CT and multimodal PET-CT. PET detects mouse tumour uptake of radiolabelled probes. The use of this technology in mice is of moderate spatial resolution (~1 mm) but compensated by its unparallel sensitivity in detecting tumours. Standard PET technology exploits the high glucose avidity of cancer masses using labelled glucose analogs. PET capabilities are rapidly expanding to measure other functional properties of tumours, such as cellular proliferation, hypoxia and apoptosis.

CT allows visualization of anatomical structures with high resolution (~50 μm) but the ability to identify tumours greatly depends on the differential absorption of radiation between the tumour and its surrounding tissue. The combination of PET and CT overcomes the intrinsic limitations of each technology, combining the high sensitivity of PET and high resolution of CT and offering an unprecedented ability to identify tumours, their functional status and dynamics.

These modalities greatly facilitate the translation of preclinical studies to applications in the clinic.

Overall, cancer researchers investigating a wide variety of targets and mechanisms of action will likely want access to both of these technologies to evaluate candidate absorption, distribution, metabolism, excretion and toxicology characteristics.

The results obtained so far from leading researchers around the world prove that we're taking preclinical molecular imaging to a new level of performance. In our group we have assessed the importance of parameters that are critical when imaging cancer in mice using CT, PET and Combined PET-CT. Adherence to a very careful handling of the mice while carrying out the study is of key importance since the mice may undergo unusual situations which may turn out to be fatal for them.

It is also essential that each study be customized to the specific mouse strain or genetically-modified mouse cohort being analyzed, adapting fasting, times and dosages of the anesthetics. Maintenance of body temperature and other vital constants are also fundamental, as is the monitoring of mice after anesthesia during recovery time, which is both essential for their wellbeing as well as a successful outcome. Handling of the mice has a profound impact on ^{18}F-FDG biodistribution and significantly influences tumour visualization. Varying the fasting state, body temperature, and mode of anesthesia may affect ^{18}F-FDG uptake in normal organs by one order of magnitude and in tumours by a factor of 3.7-x fold.

The influence of blood glucose and insulin levels on ^{18}F-FDG biodistribution is well known. Given that ^{18}F-FDG competes with glucose for intracellular transport and phosphorylation, tumour ^{18}F-FDG uptake decreases with increasing blood glucose levels. Tumour ^{18}F-FDG uptake and image contrast are lower in the non-fasted state (high insulin and glucose levels) than in the fasted state (low insulin and glucose levels).

As longitudinal studies progress through time so does tumour development and the health status of the mice deteriorates progressively. At the beginning of the studies we have to optimize all the acquisition parameters so that the tumour quantification results obtained are not altered. We have to anticipate similar situations throughout the study since the quality of life of the mice will worsen as the longitudinal study progresses.

COMUNICACIÓN INVITADA

Influence of packaging on food safety: Analytical challenges

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Food contact materials have been recognized as potential source of contaminants for food, as it has been admitted that most of the compounds having molecular weight below 1000 amu can migrate from the material to the food in contact with them. To guaranty the food safety, the legislation either in Food and Drug Administration (FDA), Japan, Australia, Mercosur and European Union (EU) regulate the chemical substances that could be used to produce the materials in contact with food and limit the maximum concentration that they could have either in the material or in the food. Most materials are regulated, including any kind of plastics, glass, ceramic, metals, regenerated cellulose as well as those currently used for specific applications such as the gaskets or lids for hermetic glass jars or the lacquers used to cover the internal side of cans, among others. Although there is a long list of chemical substances and consequently a wide series of compounds to be checked in both the materials and the food in contact with them, the control of the materials in contact with food is still a challenge, as new materials, new compounds to provide new functionalities as well as the current changes in the competitive market of food packaging materials add many difficulties to this kind of job.

The first problem to point out is the lack of knowledge about the composition of the materials, as it is not declared by the manufacturers. Thus, screening procedures are required at very low concentration level, initially in the packaging material and further in the food. Sometimes the migration takes place from an unexpected layer, which is not designed for being in direct contact with the food, as happens for example with the printing inks, adhesives or secondary packaging. There are also likely interactions between different components of the given formula, for example in adhesives, printing inks and varnishes, which result in new and unexpected migrants in the final packaging. This fact is sometimes even unknown by the producers of the materials. This situation opens another issue, such as the presence of Non Intentionally Added Substances (NIAS), which has been included as well in the EU legislation and it poses an even more challenging task.

The aim is not only to identify and quantify the migrants in the food, but also to know where they are coming from in order to remove them from the packaging material. As the maximum established limits of specific migration are often very low, of only some ng g-1 in food, it is essential to be sure that there is not crossed contamination or analytical artifacts, which would invalidate the final results.

It is clear that all these problems require analytical procedures, able to detect and quantify many different compounds in difficult matrices. The strategies and several approaches to cope with them will be shown and discussed with the help of some illustrative examples.

COMUNICACIÓN INVITADA

Protein Chips for Biomarker and Drug Discovery

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Now that the human genome has largely been sequenced, one of the most important pursuits is to understand the function of proteins it encodes. Despite immense progress in molecular biology and genetics, only a small fraction of the proteome is understood at the biochemical level. Systems biology and proteomics strive to create detailed predictive models for molecular pathways based upon the quantitative behavior of proteins. Understanding these dynamic networks provides clues into the consequence of aberrant interactions and why they lead to diseases like cancer. However, collecting biochemical data about protein behavior at scale has been daunting. Historically, methods capable of collecting quantitative data on biochemical interactions could only be used for one or a few proteins at the time. Here, we show the combination of two technologies that together could lead to the ability to measure binding events in real time for many protein interactions simultaneously using a label free technology. This could revolutionize the study of protein interactions networks by enabling quantitative comparisons of binding affinities across many molecular species, as well determining the kinetics rates of binding and release.

The first technology is protein microarrays, which display thousands of proteins in high density and enable their simultaneous biochemical characterization. We use Nucleic Acid Programmable Protein Arrays (NAPPA), as a method for producing the microarrays, because they replace the complex process of spotting purified proteins with the simpler process of spotting plasmid DNA. The proteins can then be simultaneously transcribed/translated *in situ* at the time of the assay. The second technology is a surface plasmon resonance imaging (SPRi) device that has been adapted to multiplexed binding events from a planar surface and is compatible with the protein microarray. In addition this technique is sensitive, accurate and provides real-time date for both the equilibrium and the interaction kinetics. The project is focused at coupling NAPPA protein array technology to multiplexed realtime label-free SPRi-based detection system (which allows thousands of binding events to be monitored in real-time without any loss in sensitivity). By SPR*i* we were able to detect binary interactions using NAPPA format. The combination of both technologies allows us to generate detailed kinetic data of interaction pathways.

COMUNICACIÓN INVITADA

Antidoping control, cross road between Chemistry and other Life Sciences

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Most of the compounds included in the list of prohibited drugs in human and animal sports are low molecular weight compounds. The detection of their misuse is performed through the analysis in biological samples (mainly urine) of the parent compounds or their metabolites. The metabolism of the compounds has to be known in order to identify the best markers to detect their administration. In antidoping control, chemical screening methods addressing groups of compounds with similar physicochemical properties are applied to all samples to eliminate "true negative" specimens. For first-round suspicious samples, a confirmation method based on mass spectrometry (MS), specific for the compound detected, is applied. Gas or liquid chromatography coupled to MS are the most used techniques. Due to the stringent requirements in sensitivity and specificity, high performance chromatography coupled to high resolution MS or tandem MS (MS-MS) is applied for some compounds.

However, another relevant challenge nowadays is to detect those doping substances available thanks to biotechnological advances that bear the same (or nearly the same) structure than the endogenous counterparts. To face this issue requires a deep overlapping between chemistry and other established methodologies in life sciences.

In this regards, erythropoietin is one of the most powerful doping agents although its detection by differentiating the recombinant variants from the endogenously produced hormone is one of the most demanding challenges. An important focus was set on the structural elucidation of the variability of the protein structure with particular attention to the glycans.

Growth hormone (GH) is also an active playground for the anti-doping research. Over the last decade substantial efforts were put into the development of analytical protocols for this family of compounds. Based on the philosophy that the relatively stable endogenous ratio between isoforms should be altered through the administration of a single recombinant pharmaceutical, differential immunoassays have been succesfully developed. In this approach where the ratio between the 22 kDa and all pituitary variants is determined, precise knowledge on the relative avidity and affinity of each antibody to different isoforms was established by means of surface plasmon resonance, thus facilitating the precise interpretation of immunoassays results. Also related with GH, the synthetic growth hormone Secretagogues (ghrelin analogs and mimetics) which target the GHS-1a receptor have been studied. A protocol based on the displacement of labeled ghrelin from incubations with receptor expressing cells is being developed. This time, the analytical protocol will be in place even before any doping attempt by those compounds.

As evident from the above paragraphs, challenges in sports drug testing come from different areas, and science will need to cope with them. For instance, the use of blood transfusion, especially the so-called autologous transfusion. In this regards, indirect markers, such as the unexpectedly high concentrations of phthalates in urine (leaking from the plastic materials of the bags containing blood) are becoming useful to identify potential cheaters.

New analytical advances shall be implemented, mainly on MS and nanotechnologies. Also permanent surveillance of pharmaceutical developments that may be misused in sport, is mandatory. However, the biggest challenge for the next decade may come probably from the application of the so-called gene doping, which gives rise to the *in vivo* expression of a performance enhancing hormone in commonly non-expressing

human tissues. Next years will also see an increment in the longitudinal follow-up of individual athletes (biological passport) to rapidly identify any unnatural deviation of key biochemical parameters.

SESIÓN DE PÓSTERS – LUNES 14 DE NOVIEMBRE

Medio Ambiente
Automatización y Miniaturización
Nanotecnología
Desarrollo en Instrumentación Analítica

Medio Ambiente

MAM-P01 M. Alier Pedemonte ; B.L. van Drooge ; M. Dall'Osto ; R. Tauler ; J.O. Grimalt

ORGANIC COMPOUND ANALYSIS AND CHEMOMETRIC STUDY IN URBAN FINE PARTICULATE MATTER (PM1)

P02 D. Almarcha ; J. Caixach Gamisans

COMPARISON OF SLE, SPME AND THERMAL DESORPTION FOR SEMI-QUANTITATIVE VOC SCREENING IN AIR EMISSIONS FROM ENVIRONMENTAL TREATMENT FACILITIES

P03 L. Almela ; P. Andreo ; P. Almela ; C. Veracruz ; A. Valero ; L. Coll ; J.A. Albaladejo

MS/MS *VS*
YCHLORINATED DIOXINS AND FURANS

P04 M. Alonso; A. Godayol ; E. Anticó ; J.M. Sanchez

NEEDLE-TRAP ANALYSIS OF PRIORITY VOLATILE ORGANIC COMPOUNDS FROM NATURAL AND WASTEWATER SAMPLES: EVALUATION OF DIFFERENT SAMPLING PROCEDURES

P05 M. Alonso Castillo ; I. Sánchez Trujillo ; A. García de Torres ; E. Vereda Alonso ; J.M. Cano Pavón
DETERMINATION OF TRACE PB IN SEA–WATER BY SOLID PHASE EXTRACTION COUPLED WITH FI-HG-ETAAS

P06 I. Aparicio Gómez ; J. Martín ; D. Camacho-Muñoz ; J.L. Santos ; E. Alonso

MAM-P07

MAM-P08

MAM-P09

MAM-P10 Pérez ; M.M. Afonso ; J.A. Palenzuela ; M.A. Rodríguez-Delgado

1,3-DIPENTYLIMIDAZOLIUM HEXAFLUOROPHOSPHATE IONIC LIQUID AS A NEW EXTRACTION SOLVENT IN DISPERSIVE LIQUID-LIQUID MICROEXTRACTION: EXTRACTION

OF PESTICIDES AND METABOLITES FROM SOILS

O. Ballesteros Garcia ; C. Fernández-Ramos ; A. Zafra-Gómez ; R. Blanc ; A. Navalón ; J.L. Vílchez
DEVELOPMENT OF A LC-ESI-MS/MS METHOD FOR THE ANALYSIS OF ALCOHOL ETOXYSULFATES IN WASTEWATER TREATMENT PLANTS FROM GRANADA

E. Barrado ; K. Aguilar-Arteaga ; J.A. Rodríguez ; M.E. Páez-Hernández ; C. Díez

MAGNETIC SOLID PHASE EXTRACTION FOLLOWED BY HPLC FOR ANALYSIS OF ATRAZINE AND SIMAZINE IN WATER SAMPLES

R.S. Barranquero ; M. Varni ; A. Ruiz de Galarreta

HYDROCHEMICAL ANALYSIS OF GROUNDWATER IN LANGUEYÚ CREEK BASIN, TANDIL, ARGENTINA

M.A. Barrero Mazquiarán ; M. González Aguirre ; L. Cantón

CLASSIFICATION OF ATMOSPHERIC AMBIENTS BY AEROSOL PARTICULATE PARAMETERS AND CHEMICAL COMPOSITION

R.J. Barrio ; R. Gutierrez-Climente ; A. Gómez-Caballero ; N. Unceta ; M.A. Goicolea

OPTIMIZATION OF POLY (STYRENE-CO-DIVINYLBENZENE) SYNTHESIS FOR THE DEVELOPMENT TO TAILOR-MADE HPLC COLUMNS. APPLICATION TO PESTICIDES SEPARATION

M. Beneito Cambra ; L. Ripoll-Seguer ; J.M. Herrero-Martínez ; E.F. Simó-Alfonso ; G. Ramis-Ramos
CHROMATOGRAPHIC ANALYSIS OF NON IONIC AND ANIONIC ETHOXYLATED SURFACTANTS IN CLEANING PRODUCTS

M.R. Boleda Vall-llovera ; M.T. Galceran ; F. Ventura

ANALYSIS OF 44 SELECTED PRIORITY PHARMACEUTICALS IN WATERS AT TRACE LEVELS BY AN ON-LINE SPE LIQUID CHROMATOGRAPHY TANDEM MASS PECTROMETRY MULTIRESIDUE METHOD

G. Bolívar Subirats ; H. Gallart-Ayala ; E. Moyano ; M.T. Galceran

UHPLC-MS/MS FOR THE MONITORING OF GIBBERELLINS AT DIFFERENT GROWTH STAGES IN FRUIT TREES

C. Caballo Linares ; M.D. Sicilia Criado ; S. Rubio Bravo

STEREOSELECTIVE DETERMINATION OF MECOPROP AND DICHLORPROP IN NATURAL WATERS BY SUPRAMOLECULAR SOLVENT-BASED MICROEXTRACTION AND LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY

C. Corcellas ; M.L. Feo ; J.P.M. Torres ; O. Malm ; W. Ocampo-Duque ; E. Eljarrat ; D. Barceló

PYRETHROIDS: NEW CONTAMINANTS IN HUMAN BREAST MILK

E. Cirera-Domènech ; F. Broto-Puig ; C. Ribas-Font ; L. Comellas-Riera ; S. Paz-Estivill ; R. Delgado-Ortiz
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J. Silva Felix ; C. Domeño ; C. Nerín

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N. Caballero Casero ; S. García-Fonseca ; S. Rubio

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E. Canellas Aguareles ; P. Vera ; C. Domeño ; P. Alfaro ; C. Nerín

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S. Capel Cuevas ; N. López Ruiz ; A. Martínez Olmos ; M.P. Cuéllar ; M.C. Pegalajar ; I. de Orbe-Payá ; A.J. Palma ; L.F. Capitán-Vallvey
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D. Company Arumi ; M. Figueras ; V. Salvadó ; M. Molinas ; O. Serra ; E. Anticó

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A GAS CHROMATOGRAPHY - MASS SPECTROMETRY METHOD FOR THE SIMULTANEOUS DETERMINATION IN PERFUMES OF THE PHTHALATES BANNED BY THE EUROPEAN COSMETIC PRODUCTS REGULATION

Correcciones de erratas detectadas:

López Mesas, L., MAM-OC01
Kharim, K., AYM-P06
Martín-Álvarez, J.P., OAI-OC03