



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
GRANADA, 21 - 24 JUNE 2010



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

## **POSTER COMMUNICATIONS: SESSION #1**

### **PO1-01 APPLICATION OF EXPERIMENTAL DESIGN AND DESIRABILITY FUNCTION FOR THE SIMULTANEOUS EXTRACTION OF PESTICIDES FROM AQUEOUS SAMPLES BY SOLID PHASE MICROEXTRACTION**

A. Garrido Frenich, J. L. Martínez Vidal, R. Martínez Ocaña, P. Baquero Fera, R. Romero-González, M. M. Martín Fernández

### **PO1-02 OPTIMISATION OF A HEADSPACE SOLID-PHASE MICROEXTRACTION METHOD FOR THE DIRECT DETERMINATION OF VOLATILE PHENOLS IN CIDER**

C. Pizarro, N. Pérez-del-Notario, J.M. González-Sáiz

### **PO1-03 USE OF MAIN MINERAL ELEMENTS COUPLED WITH LINEAL DISCRIMINANT ANALYSIS TO DIFFERENTIATE BETWEEN ORGANIC AND NON ORGANIC HARD EWE CHEESE**

M. I. González-Martín, J. M. Hernández-Hierro, I. Revilla, A. Vivar-Quintana, C. González-Pérez, I. A. Lobos Ortega

### **PO1-04 UNSUPERVISED GROUPING OF VALERIANA OFFICINALIS BY HPLC-DAD AND PARAFAC2 MODELING**

J. R. Lucio-Gutiérrez, J. Coello, S. MasPOCH, J. M. Amigo

### **PO1-05 COMPOUND COLOR RECOGNITION VIA IMAGE ANALYSIS ON HIGH THROUGHPUT SCREENING COMPOUND LIBRARIES**

M. von Korff, J. Freyss, A. Klenk, J. Silva, G. Bourquin, O. Peter, T. Sander

### **PO1-06 PRINCIPAL COMPONENT ANALYSIS FOR VERY LARGE DATA SETS**

J. Camacho, J. Díaz-Verdejo

### **PO1-07 AUTOMATED DLLME METHOD FOR THE DETERMINATION OF CORK TAIN RESPONSIBLE COMPOUNDS IN WINE**

C. Pizarro, J.M. González-Sáinz, C. Sáenz-González, N. Pérez-del-Notario

### **PO1-08 BLEND UNIFORMITY STUDY OF POORLY MISCIBLE AND LOW DOSE POWDERS BY NEAR-INFRARED SPECTROSCOPY**

M. Blanco, R. Cueva-Mestanza

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO1-09 D-OPTIMAL DESIGN AND THE SECOND ORDER PROPERTY TO OPTIMIZE A SPE PROCEDURE TO ANALYZE TRIAZINES IN INFUSIONS BY GC-MS**

B. D. Real, M.C. Ortiz, L.A. Sarabia

**PO1-10 MULTIVARIATE ANALYSIS TO STUDY THE RELATION BETWEEN SENSORY AND PHYSICO-CHEMICAL VARIABLES DURING THE GRAPE MATURITY IN THE 'D.O. RIOJA'**

E. Meléndez, M.C. Ortiz, L.A. Sarabia, M. Íñiguez

**PO1-11 QUANTITATIVE DETERMINATION OF API AND EXCIPIENTS IN LORAZEPAM TABLETS BY USING NIR-HYPERSPECTRAL IMAGE AND MCR-ALS.**

F. Franch-Lage, J. M. Amigo, E. Skibsted, S. MasPOCH, J. Coello

**PO1-12 PREDICTION OF TOTAL AND VOLATILE ACIDITY IN RED WINES BY FT-IR SPECTROSCOPY AND ITERATIVE PREDICTOR WEIGHTING (IPW)**

C. Pizarro, J.M. González-Sáiz, I. E. Díez, P. Orio

**PO1-13 APLICACIÓN DEL DISEÑO ESTADÍSTICO DE EXPERIMENTOS AL DESARROLLO DE FORMULACIONES DETERGENTES**

E. Jurado Alameda, V. Bravo, R. Bailón, J. Nuñez-Olea, D. Altmajer Vaz.

**PO1-14 MORE THAN TWENTY YEARS OF CHEMOMETRICS IN RESEARCH AND TEACHING WITH 'PARVUS'**

L.A. Sarabia, M.C. Ortiz, M. S. Sánchez, A. Herrero, C. Reguera

**PO1-15 CONTROL IN-SITU OF OLIVE MATURITY FOR PRODUCTION OF OLIVE OIL BY NEAR INFRARED SPECTROSCOPY (NIRS)**

M. Ybarra-Lalor, A.J. Fernández-Espinosa, R. Bouza-Deaño, M. Ternero-Rodríguez

**PO1-16 QUALITY CONTROL OF LUBRICANTS BY NIR SPECTROSCOPY**

M. Blanco, D. Zamora, M. Bautista, R. Mulero, M. Mir

**PO1-17 FLATBED SCANNERS AS A SOURCE OF IMAGE FOR EXPLORING THE QUALITY OF NICKEL-ELECTROPLATING DEPOSITS**

J.M. Amigo, R. Bro, M. Ostra, C. Ubide, M. Vidal

**PO1-18 EXPERIMENTAL DESIGN APPLICATION FOR TRIAZOLE FUNGICIDES DETERMINATION IN FOOD LIQUID SAMPLES BY SOLID-PHASE MICROEXTRACTION AND GC-ECD**

A. Bordagaray, E. Millán, R. Garcia Arrona

**PO1-19 NEW METHODOLOGY OF THE TREATMENT OF DATA IN COMPUTACIONAL CHEMICAL KINETICS**

M.M. Canedo Alonso, J.L. González Hernández

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO1-20 AZA-MICHAEL REACTION WITH MODIFIED VEGETABLE OILS. EVIDENCE OF THE KETO-ENOLIC EQUILIBRIUM WITH NIR-CHEMICAL IMAGING AND EVOLVING FACTOR ANALYSIS**

I..Martí-Aluja, I. Ruisánchez, V. Cádiz, S. Maspoch M.S. Larrechi

**PO1-21 PARTICLE SIZE DETERMINATION IN PHARMACEUTICAL POWDERS BY NEAR INFRARED SPECTROSCOPY (NIRS)**

M. Sarraguça, A. Cruz, H. Amaral, P. Costa, J. Lopes

**PO1-22 MICROWAVE ASSISTED ACID DIGESTION OF BIOMORPHIC CERAMIC OBTAINED FROM BEECH WOOD INFILTRATED WITH NICKEL OXIDE: FACTORIAL DESIGN**

F. Sánchez Rojas, C. Bosch Ojeda, J.M. Cano Pavón

**PO1-23 DETERMINATION OF TRACE ELEMENTS IN NANOPERM ALLOYS BY ATOMIC ABSORPTION SPECTROMETRY**

F. Sánchez Rojas, C. Bosch Ojeda, J.M. Cano Pavón

**PO1-24 SYNTHESIS, CHARACTERIZATION AND DISSOLUTION OF BIOMORPHIC COMPOUNDS BASED ON IRON OXIDE**

C. Bosch Ojeda, F. Sánchez Rojas, J.M. Cano Pavón

**PO1-25 EXPERIMENTAL DESIGN IN THE OPTIMIZATION OF A MICROWAVE ACID DIGESTION PROCEDURE FOR THE DETERMINATION OF METALS IN BIOMORPHIC CERAMIC SAMPLES BY ICP-MS**

C. Bosch Ojeda, F. Sánchez Rojas, J.M. Cano Pavón

**PO1-26 DETERMINATION OF BASIC DENSITY IN WOODCHIPS WITH DIFFERENT MOISTURE CONTENTS USING NIR SPECTROSCOPY**

L. B. L. R. Nascimbem, B. R. Rubini, A. F. Caldeira, R. J. Poppi

**PO1-27 CALCULATION OF THE SIMILARITY BETWEEN IMAGES USING FAST NIR-CI AND CHEMOMETRIC TOOLS: APPLICATION TO CARBAMAZEPINE DRUG**

G. Post Sabin, W.F. de Carvalho Rocha, R.J. Poppi

**PO1-28 APPLICATION OF MONTE CARLO METHODOLOGY FOR THE ESTIMATION OF THE UNCERTAINTY IN A GLOBAL MIGRATION ASSAY.**

J. M. Veiga, V. Carbonell, C. Calatayud

**PO1-29 COMPARATIVE PROCESSING OF HPLC-MS DATA ORIENTED TO THE IDENTIFICATION OF BIOACTIVE COMPOUNDS IN COMPLEX SAMPLES**

S. Mota, A. de la Torre, R. Quirantes-Piné, A. Segura-Carretero, A. Fernández-Gutiérrez

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

## **PO1-30 NOISE REDUCTION ALGORITHM FOR MASS SPECTROMETRY DATA FILES**

A.de la Torre, S. Mota, C. Roldán, S. Fernández-Arroyo, A. Segura-Carretero, A. Fernández-Gutiérrez

## **PO1-31 AUTOMATIC ALIGNMENT OF MASS SPECTROMETRY DATA BASED ON GRADIENT DESCENT**

A.de la Torre, C. Benítez, C. Roldán, R. Quirantes-Piné, A. Segura-Carretero, A. Fernández-Gutiérrez

## **PO1-32 DEREPLICATION BASED ON CORRELATION BETWEEN SPECTROMETRIC DATA AND BIOACTIVITY FOR THE IDENTIFICATION OF BIOACTIVE COMPOUNDS IN PLANT EXTRACTS**

A.de la Torre, J. Menéndez, C. Roldán, A. Segura-Carretero, A. Fernández-Gutiérrez

## **PO1-33 APPLICATIONS OF PARTICLE SWARM OPTIMIZATION (PSO) TO CHEMOMETRIC PROBLEMS**

F. Marini, B. Walczak

## **PO1-34 EVALUATION OF THE EXTENT OF ROTATION AMBIGUITIES IN MULTIVARIATE CURVE RESOLUTION SOLUTIONS**

R. Tauler, J. Jaumot.

## **PO1-35 METHODOLOGY FOR THE OPTIMISATION OF EDIBLE FILMS BASED ON DESIGN OF EXPERIMENTS**

A. Pascual-Benlliure, M.J. Fabra, P. Talens, J.M. Prats-Montalbán

## **PO1-36 OPTIMIZATION OF ANALYTICAL PROCEDURE BY MEANS EXPERIMENTAL DESIGN TECHNIQUES**

C. Baschieri, L. Bertacchini, M. Cocchi, A. Marchetti, C. Durante

## **PO1-37 DEVELOPMENT AND VALIDATION OF ANALYTICAL METHOD USING MULTIVARIATE TECHNIQUES FOR OPTIMIZATION OF THE PARAMETERS INVOLVED IN HYDRIDE GENERATION**

S.M. Macedo, E.G.P. da Silva, R. M. de Jesus, W.N.L. dos Santos, S.L.C. Ferreira, J.B. de Andrade

## **PO1-38 AN AUTOMATED APPROACH FOR THE QUALITY EVALUATION OF BREAD WHEAT**

G. Foca, R. Caramanico, N. Sinelli, M. Mariotti, M. Lucisano, A. Pagani, A. Ulrici

## **PO1-39 PARTIAL LEAST-SQUARES CALIBRATION IN THE ANALYSIS OF TRACE METALS IN NATURAL WATER BY ADCSV USING PYRIDOXAL SALICYLOYLHYDRAZONE**

A. Aouarram, M.D. Galindo-Riaño, M. García-Vargas, E. Espada-Bellido

## **PO1-40 HYPERSPECTRAL IMAGING FOR PEACH RIPENING ASSESSMENT**

L. Lleó, B. Diezma-Iglesias, J.M. Roger, A. Herrero-Langreo



# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
GRANADA, 21 - 24 JUNE 2010



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO1-41 APPLICATION OF STATISTICAL DESIGNS OF EXPERIMENT WITH DESIRABILITY FUNCTION FOR THE EXTRACTION OF MULTIRESIDUE PESTICIDES FROM SEAWEED SAMPLES**

A.M. Carro, D. Garcia, R.A. Lorenzo, R. Cela

**PO1-42 DIRECT ORTHOGONALIZATION K-NEAREST NEIGHBOURS**

J.L. Villa, J. Ferré, R. Boqué

**PO1-43 EVALUATION OF THE PHYTOTOXICITY AT ABANDONED MINING SITE USING PRINCIPAL COMPONENT ANALYSIS**

C. Estepa Molina, P. de la Mata Espinosa, M.G. Bagur González, S. Morales Ruano, F. Martín Peinado.

**PO1-44 ASSESSMENT OF THE SEQUENTIAL PRINCIPAL COMPONENT ANALYSIS (SPCA) CHEMOMETRIC TOOL TO IDENTIFY THE SOLUBLE ATMOSPHERIC POLLUTANTS IN RAINWATERS**

R. Montoya Mayor, A.J. Fernández Espinosa, M. Ternero Rodríguez

**PO1-45 VALIDATION OF A METHOD FOR ANION DETERMINATION IN WASTEWATER. ESTIMATING OF MEASUREMENT UNCERTAINTY**

M. Hernández Revilla, M. Vega Alegre

**PO1-46 MINIMISATION OF INSTRUMENTAL NOISE IN THE ACQUISITION OF FT-NIR SPECTRA OF BREAD WHEAT USING EXPERIMENTAL DESIGN AND SIGNAL PROCESSING TECHNIQUES**

A. Ulrici, C. Ferrari, N. Sinelli, M. Mariotti, M. Corbellini, G. Foca

**PO1-47 COMPUTER-ASSISTED OPTIMIZATION OF HIGH-TEMPERATURE LIQUID CHROMATOGRAPHIC SEPARATIONS**

J. García-Lavandeira, P. Oliveri, M. Forina, R. Cela

**PO1-48 FUNCIONAL ANALYSIS OF CHEMOMETRIC DATA**

A.M. Aguilera, M. Escabias, M.J. Valderrama y M.C. Aguilera-Morillo

**PO1-49 DISCUSSION OF DETECTION LIMIT ESTIMATION IN LOGARITHMIC CALIBRATIONS FOR ELECTROCHEMILUMINESCENT BIOSENSORS**

J. Ballesta-Claver, M. C. Valencia-Mirón, L. Cuadros Rodríguez, L.F. Capitán-Vallvey

**PO1-50 NIR MONITORING OF PELLETS MANUFACTURING: AN EXAMPLE OF PROCESS ANALYTICAL TECHNOLOGY IN THE PHARMACEUTICAL INDUSTRY**

M. Alcalà, M. Blanco, F. Santamaría, M. Garcia

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*

**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO1-51 OBTAINING INFORMATION FROM A BIOSYNTHETIC PATHWAY USING MULTI-WAVELENGTH FLUORESCENCE SPECTROSCOPY AND CHEMOMETRIC TOOLS**

R. C. Dantas Muniz Filho, M. P. Reis Melo, N. Duràn, P. L. Onófrio Volpe, R. Tauler, M. M. Castro Ferreira

**PO1-52 THE FORENSIC ANALYSIS OF SOIL BY FTIR WITH MULTIVARIATE ANALYSIS**

T. Atherton, M. Baron, R. Croxton, J. Gonzalez-Rodriguez, R. Gonzalez, R. Jimenez

**PO1-53 IMAGE FEATURE SELECTION IN WT DOMAIN: COUPLING 2D FAST WAVELET TRANSFORM AND GENETIC ALGORITHMS**

M. Cocchi, M. Demartini, E. Marengo

**PO1-54 PREDICTION OF DESTRUCTIVE PROPERTIES USING DESCRIPTIVE ANALYSIS OF ND MEASUREMENTS**

A.Herrero-Langreo, E. Fernández-Ahumada, J.M. Roger, B. Palagos, L. Lleó

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
GRANADA, 21 - 24 JUNE 2010



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

## **POSTER COMMUNICATIONS: SESSION #2**

### **PO2-01 DETERMINATION OF MARKER PTERIDINS IN URINE BY HPLC WITH FLUORIMETRIC DETECTION AND SECOND-ORDER MULTIVARIATE CALIBRATION USING MCR-ALS.**

A. Muñoz de la Peña, A. Espinosa, F. Cañada, A. Mancha, H. Goicoechea, M. de Zan, J. Culzoni.

### **PO2-02 API DETERMINATION BY NIR SPECTROMETRY. A NOVEL APPROACH TO CONSTRUCT A CALIBRATION SET WITHOUT REFERENCE METHOD**

A. Peguero, M. Blanco

### **PO2-03 CLASSIFICATION OF BEERS USING QUALITY CONTROL PARAMETERS**

A. Alcázar, J. M. Jurado, M.J. Martín, F. Pablos

### **PO2-04 VARIABLE SELECTION FOR MULTIFACTORIAL GENOMICS DATA**

S. Tarazona, S. Prado López, A. Ferrer, A. Conesa

### **PO2-05 AUTHENTICATION OF FATTENING DIET OF IBERIAN PIG ACCORDING TO THEIR VOLATILE PROFILE FROM SUBCUTANEOUS FAT**

M. Narváez-Rivas, M. León-Camacho, J. M. Jurado, F. de Pablos

### **PO2-06 EVALUATION OF THE POTENCIAL OF QUALITY PARAMETERS, UNSPECIFIC UV-VIS PROFILES AND THE SYNERGY EFFECT ON THE CLASSIFICATION OF SPANISH EXTRA VIRGIN OLIVE OILS**

C. Pizarro, J.M. González-Sáiz, S. Rodríguez-Tecedor, I. Rodríguez-Artieta, N. Pérez-del-Notario

### **PO2-07 INVESTIGATION OF THE SOURCE COMPOSITION AND SPATIAL DISTRIBUTION OF THE VOCS MEASURED ALONG THE GALICIAN COAST (NW SPAIN) AFTER THE PRESTIGE OIL SPILL USING CHEMOMETRIC METHODS**

C. Pérez-Rial, R. Tauler, P. López-Mahía, S. Muniategui-Lorenzo, D. Prada-Rodríguez

### **PO2-08 COMPARING DIFFERENT 3-WAY DECOMPOSITION METHODS APPLIED TO ROADSOILS POLLUTION**

M.P. Gómez-Carracedo, D. Ballabio, J.M. Andrade, R. Fernández-Varela, J. Aires-de-Sousa, R. Todeschini

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*

**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO2-09 USE OF SELF ORGANIZING MAPS WITH POLYCYCLIC AROMATIC HYDROCARBONS 3-WAY DATA FROM SPILLED OILS**

R. Fernández-Varela, M.P. Gómez-Carracedo, J.M. Andrade, D. Ballabio, V. Consonni, R. Todeschini

**PO2-10 PATTERN RECOGNITION OF POLYCYCLIC AROMATIC HYDROCARBONS MEASURED ON GALICIAN COASTAL WATERS AFTER THE PRESTIGE'S WRECK**

G. Grueiro-Noche, J.M. Andrade, S. Muniategui-Lorenzo, P. López-Mahía, D. Prada-Rodríguez

**PO2-11 3-WAY PATTERN-RECOGNITION OF PAHS FROM CANTABRIA (N SPAIN) SEAWATER SAMPLES**

G. Grueiro-Noche, J.M. Andrade, S. Muniategui-Lorenzo, P. López-Mahía, D. Prada-Rodríguez

**PO2-12 CHEMOMETRIC STUDY OF AZO DYES PHOTODEGRADATION USING UV-VIS SPECTRAL DATA**

C. Fernández, M. P. Callao, M. S. Larrechi

**PO2-13 SEQUENTIAL INJECTION ANALYSIS FOR THE DETERMINATION OF SULFATE IN WATER USING SECOND-ORDER DATA**

V. del Río, M.S. Larrechi, M.P. Callao

**PO2-14 PEROXYL RADICAL SCAVENGING AND HYDROXYL RADICAL PREVENTION CAPACITY OF SOME PHENOLIC ACIDS**

M. López- Vélez, F. Martínez-Martínez

**PO2-15 CHEMOMETRIC EVALUATION OF THE EFFECTS OF DIFFERENT TYPE OF CULTURES ON WHEAT DEVELOPMENT UNDER DIFFERENT EXPERIMENTAL CONDITIONS USING LC-MS-DAD PROFILES**

M. Farrés, M. Villagrasa, E. Eljarrat, D. Barceló, R. Tauler

**PO2-16 TRILINEARITY AND COMPONENT INTERACTION CONSTRAINTS IN THE MULTI-VARIATE CURVE RESOLUTION INVESTIGATION OF NO AND O3 POLLUTION IN BARCELONA**

M. Alier, M. Felipe, I. Hernández, R. Tauler

**PO2-17 IDENTIFICATION OF CONTAMINATION SOURCES IN ESTUARINE WATER BY MULTIWAY DATA ANALYSIS. A CASE OF STUDY: ESTUARY OF THE NERBIOI-IBAIZABAL RIVER**

A.Gredilla, J.M. Amigo, S. Fdez-Ortiz de Vallejuelo, A. de Diego, R. Bro, J.M. Madariaga

**PO2-18 FAST ANALYSIS OF SOME PHENOLICS BY HPLC-DAD AND CHEMOMETRIC RESOLUTION TECHNIQUES**

F. Marini, R. Nescatelli, F. Balestrieri, R. Bucci, A. L. Magri, A.D. Magri



# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO2-19 RECOGNITION OF METABOLIC PATTERNS IN KIDNEY TRANSPLANTED PATIENTS BY NMR ELABORATION OF NMR PROFILE DATA**

M. Calderisi, A. Vivi, M. Tassini, M. Cocchi, M. Carmellini, R. Madsen, J. Trygg

**PO2-20 AROMATIC CHARACTERIZATION AND CLASSIFICATION OF BEER SAMPLES BY MEANS OF MS E-NOSE AND CHEMOMETRIC TOOLS**

L. Vera, M. Mestres, R. Boqué, J. Guasch, O. Busto

**PO2-21 MONITORING THE PHENOLIC EXTRACTION ON RED WINE FERMENTATIONS USING FT-IR SPECTROSCOPY AND MULTIVARIATE ANALYSIS**

S. Fragoso, M. Mestres, R. Boqué, J. Guasch, O. Busto

**PO2-22 A COMPARISON BETWEEN CLASSICAL AND INNOVATIVE CLASS-MODELLING TECHNIQUES FOR THE CHARACTERISATION OF A PDO OLIVE OIL**

P. Oliveri, M. Casale, M.C. Casolino, M. Forina

**PO2-23 USE OF PRINCIPAL COMPONENT ANALYSIS AND HIERARCHICAL CLUSTER ANALYSIS FOR EVALUATION OF THE MINERAL COMPOSITION WATERCRESS**

A.M.P. dos Santos, H.C. de Souza, S. L.C. Ferreira, D. M.N. Fortunato, D.C. Lima, W.D. Fragoso

**PO2-24 APPLICATION OF THREE-WAY TUCKER ANALYSIS TO STUDY DISTRIBUTION OF HEAVY METAL CONTAMINATION IN FISH FROM CADIZ GULF**

J.J. Vicente-Martorell, M.D. Galindo-Riaño, J.A. López-López, M. García-Vargas

**PO2-25 ASSESSMENT OF THE METAL POLLUTION, POTENTIAL TOXICITY AND SPECIATION OF SEDIMENT FROM ALGECIRAS BAY (SOUTH OF SPAIN) USING CHEMOMETRIC TOOLS**

C.M. Kosore, M.D. Galindo-Riaño, M.J. Casanueva-Marenco, M. García-Vargas, M. Díaz-de Alba

**PO2-26 APPLICATION OF TWO- AND THREE-WAY PRINCIPAL COMPONENT ANALYSIS TO THE STUDY OF METAL CONTAMINATION FROM MINING WASTES**

M. Sánchez, M. Hidalgo, R. Tauler

**PO2-27 DEFINING SENSORY DESCRIPTORS OF PARMIGIANO REGGIANO CHEESE BY COMBINING A RING-TRIAL AMONG SENSORY LABORATORIES AND MULTIVARIATE STATISTICAL ANALYSIS**

C.Giussani, S. Roncoroni, M. Zannoni, L. Galassi, A. Garavaldi, M. Turrini

**PO2-28 CHEMICAL AND ISOTOPIC TRACERS IN COPPER DEPOSITS AND ANCIENT ARTEFACTS: A MULTIVARIATE ANALYSIS APPROACH TO ESTABLISH THE PROVENANCE OF MATERIALS**

B. Giussani, M. Marelli, S. Recchia, S. Roncoroni, I. Angelini, G. Artioli, I. Giunti

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**P02-29 BROAD-RANGE OPTICAL pH SENSOR BASED ON NEURAL NETWORKS**

S. Capel-Cuevas, M.P. Cuéllar, I. de Orbe-Payá, M.C. Pegalajar, L.F. Capitán-Vallvey

**P02-30 MINIMIZATION OF SENSING ELEMENTS FOR BROAD-RANGE OPTICAL PH DEVICE FORMULATION**

S. Capel-Cuevas, M.P. Cuéllar, I. de Orbe-Payá, M.C. Pegalajar, L.F. Capitán-Vallvey

**P02-31 PARAFAC AND D-OPTIMAL DESIGN TO OPTIMIZE A PROCEDURE TO DETERMINE SULFATHIAZOLE IN MILK USING FLUORESCENCE SPECTROSCOPY**

R. Morales, M.C. Ortiz, L.A. Sarabia

**P02-32 EXPLORATORY ANALYSIS APPLIED IN THE EVALUATION OF MINERAL COMPOSITION OF NUT-COLA CONSUMED IN BAHIA STATE, BRAZIL**

V. Sales Martins, R. Mota de Jesus, S. L. Costa Ferreira

**P02-33 IMPROVING MULTIVARIATE CALIBRATION OF A DISPOSABLE OPTICAL TONGUE FOR HEAVY METAL ANALYSIS BY BOOTSTRAPPING TECHNIQUES**

M. Ariza Avidad, J. Vukovic, M.P. Cuellar, M.C. Pegalajar, L.F. Capitan-Vallvey

**P02-34 A NEURONAL NETWORK APPROACH FOR ALKALINE ION DISPOSABLE OPTICAL TONGUE**

M.M. Erenas, M.P. Cuellar, I. de Orbe-Payá, M.C. Pegalajar, L.F. Capitán-Vallvey

**P02-35 EXPLORATORY DATA ANALYSIS OF CHROMATOGRAPHIC PROFILES OF TAGS IN VARIETIES OF OLIVE OIL BY USING HT/GC- (IT)MS**

C. Ruiz-Samblás, P. de la Mata Espinosa, L. Cuadros-Rodríguez, A. González-Casado, F.P. Rodríguez García

**P02-36 CHEMICAL EQUILIBRIA STUDIES USING MULTIVARIATE ANALYSIS METHODS**

J. Jaumot, R. Eritja, A. Stępień, R. Gargallo

**P02-37 GENE SELECTION IN MICROARRAY DATA BASED ON SELECTIVITY RATIO**

C. Botella, J. Ferré, R. Boqué

**P02-38 STATISTICAL STUDY OF SOAP AND LAS IN SEWAGE SLUDGE SAMPLES**

S. Cantarero, O. Ballesteros, A. Zafra-Gómez, A. Navalón, J.L. Vílchez, M. S. Reis, P. M. Saraiva, J. De Ferrer, C. Verge

**P02-39 STATISTICAL STUDY OF SOAP AND LAS IN MARINE SEDIMENTS SAMPLES**

S. Cantarero, O. Ballesteros, A. Zafra-Gómez, A. Navalón, J.L. Vílchez, M. S. Reis, P. M. Saraiva, J. De Ferrer, C. Verge

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO2-40 POTENTIAL OF LC-ESI-TOF MS AND GC-APCI-MAXIS MS DATA TOGETHER WITH STATISTICAL TOOLS TO IDENTIFY PHENOLIC COMPOUNDS OF EXTRA-VIRGIN OLIVE OIL AS VARIETAL MARKERS**

R.García-Villalba, A.Carrasco-Pancorbo, E. Nevedomskaya, T.Pacchiarotta, O. A. Mayboroda, A. M. Deelder, A.Segura-Carretero, A. Fernández-Gutiérrez.

**PO2-41 EVALUATION OF ANTIOXIDANT CAPACITY BY TWO DIFFERENT ANALYTICAL METHODS IN SERUM SAMPLES OF PATIENTS WITH ALTERED LEVELS OF SOME TUMORAL MARKERS**

M. López- Vélez, F. Martínez- Martínez

**PO2-42 CHEMOMETRIC APPROACH: TRIACYLGLYCERIDES PROFILES IN VEGETABLE OILS BY PRINCIPAL COMPONENT ANALYSIS**

P. de la Mata-Espinosa, R.Bro, J.M. Bosque-Sendra, L. Cuadros-Rodríguez, F.P. Rodríguez-García

**PO2-43 OPTIMIZATION OF EXPERIMENTAL VARIABLES BY DOEHLERT DESIGN IN A PORTABLE OPTICAL CO<sub>2</sub> INSTRUMENTATION**

I.M. Pérez de Vargas-Sansalvador , A. Martínez-Olmos , C. Estepa-Molina , P. de la Mata-Espinosa, M.D. Fernández-Ramos, A.J. Palma , L.F. Capitán-Vallvey

**PO2-44 AGEING AND OXIDATION PROCESSES OF OLIVE OIL SAMPLES DURING STORAGE FOLLOWED BY NEAR-INFRARED SPECTROSCOPY AND ARTIFICIAL NOSE**

C. Armanino, M.C. Casolino, M. Casale, M. Forina, S. Lanteri, P. Oliveri

**PO2-45 MCR-ALS ANALYSIS OF EXCITATION EMISSION MATRICES OF FLUORESCENT NANOPARTICLES**

J.M.M. Leitão, J.C.G. Esteves da Silva

**PO2-46 POTENTIAL OF ENERGY DISPERSIVE X-RAY FLUORESCENCE AND NEAR INFRARED TECHNIQUES COUPLED WITH CHEMOMETRICS IN THE CALIBRATION OF WATER AND ALCOHOL CONTENTS IN SAMPLES OF CACHAÇA**

M.P. Reis Melo, R.C. Dantas Muniz Filho, M.I. Maretti Silveira Bueno, M.M. Castro Ferreira

**PO2-47 DETECTION AND QUANTIFICATION OF OLIVE OIL IN OIL BLENDS BY INFRARED SPECTROSCOPY**

M.J. Ayora Cañada, A. Domínguez Vidal, A.P. de la Mata Espinosa, C. Ruiz Samblás, L. Cuadros Rodríguez

**PO2-48 A CHEMOMETRIC APPROACH TO THE STUDY OF THE BINDING MEDIA COMPOSITION ON RED AND BLUE MICRO-SAMPLES FROM PORTUGUESE MEDIEVAL ILLUMINATED MANUSCRIPTS**

C. Miguel, J. A. Lopes, M.J. Melo, M. Clarke

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
**GRANADA, 21 - 24 JUNE 2010**



Web site: [www.ugr.es/~ecugr](http://www.ugr.es/~ecugr)

**PO2-49 METHOD VALIDATION OF PCA FOR ACCELERATED THERMALAGING BY INTERNAL STANDARD**

J. Romero-Pastor, A. Yebra, P. Álvarez-Lloret, A.B. Rodríguez-Navarro.

**PO2-50 MULTIVARIATE IDENTIFICATION OF EGG PROTEIN BY HPLC AMINO ACID ANALYSIS AND SIMCA**

R. Checa, E. Manzano, L.F. Capitán-Vallvey

**PO2-51 PRINCIPAL COMPONENT ANALYSIS TO STUDY HISTORICAL PAINTING MODEL SAMPLES BASED ON LINSEED OIL**

R. Ortega, N. Navas, J. Romero-Pastor, L.R. Rodríguez-Simón, R. Checa, L.F. Capitán-Vallvey, E. Manzano

**PO2-52 MULTIVARIATE APPROACH ON RAMAN SPECTROSCOPIC DATA TO INVESTIGATE PROTEIN- PIGMENT INTERACTION IN WHITE TEMPERA PAINTINGS**

N. Navas, J. Romero-Pastor, E. Manzano, C. Cardell

**PO2-53 PRELIMINARY STUDY OF UV-ACCELERATED AGEING OF POTEINACEOUS BINDIG MEDIA BY MALDI-TOF-MS AND CHEMIOMETRY TECHNIQUES**

J. Romero-Pastor, S. Kuckova, C. Cardell, E. Manzano, N. Navas

**PO2-54 A CLASSIFICATION OF FRESH OLIVE VARIETIES BY FOURIER TRANSFORM INFRARED SPECTROSCOPY ANALYSIS AND CHEMOMETRICS**

A. Oussama, W. Terouzi, A. Bolli, M. De Luca, G. Ragno