

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM



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



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## **ORAL PRESENTATIONS: SESSION #1**

### **OP1-01 OPTIMISATION OF COUNTER-PROPAGATION ARTIFICIAL NEURAL NETWORKS BY MEANS OF GENETIC ALGORITHMS**

D. Ballabio, M. Vasighi, R. Todeschini

### **OP1-02 APPLICATION OF MISSING DATA METHODS FOR EXPLORATORY DATA ANALYSIS IN MEDICAL RESEARCH**

J. Camacho, J. Bondia, J. Vehí, J.M. Fernández-Real

### **OP1-03 BATCH PROCESS USING NIR SPECTROSCOPY IN A QUALITY BY DESIGN APPROACH**

J. Rosas, M. Blanco, M. Alcalà

### **OP1-04 A CROSS-VALIDATION PROCEDURE FOR CLASS-MODELLING TECHNIQUES THAT PROVIDE A FAMILY OF OPTIMAL SOLUTIONS**

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

### **OP1-05 FUZZY COMPARISON OF BALLISTIC IMAGES**

M. Otto, K. Wilke, S. Fritzsche, K. Korndörfer, T. Liebscher, W. Wenz

### **OP1-06 MULTIVARIATE CURVE RESOLUTION APPLIED TO THE ANALYSIS OF MICRORRAY DATA**

J. Jaumot, B. Piña, R. Tauler

### **OP1-07 BIOREACTOR MONITORING WITH SPECTROSCOPY AND CHEMOMETRICS: A REVIEW**

N.D. Lourenço, J.A. Lopes, C.F. Almeida, M.C. Sarraguça, H.M. Pinheiro

### **OP1-08 CHEMOMETRIC TO INVESTIGATE AND RESOLVE SPECTROKINETIC DATA OF ULTRAFAST PHOTOINDUCED PROCESSES**

N. Mouton, B. Debus, M. Sliwa, A. De Juan, C. Ruckebusch

### **OP1-09 NIR HYPERIMAGING TECHNIQUES FOR THE EVALUATION OF GEL STRIPS IN PHARMACEUTICAL INDUSTRY**

J.M. Prats-Montalbán, J.I. Jérez-Rozo, R.J. Romañach, A. Ferrer

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**OP1-10 H-VALUE AS ANALYTICAL PARAMETER IN IMAGE ANALYSIS**

M.M. Erenas, K. Cantrell, I. de Orbe-Paya, L.F. Capitan-Vallvey

**OP1-11 MULTIDIMENSIONAL NON SUPERVISED ANALYSIS (TEXTURAL AND SPACIAL) IN MRI TOMOGRAPHY FOR WATERCORE DETECTION**

A.Melado; P. Barreiro; J. Ruíz-Cabello; M.E. Fernández-Valle; A. Blanco; J. Val, J.M. Roger

**OP1-12 MULTIVARIATE APPROACH TO DATA MINING AND DATA INTEGRATION**

L. Eriksson

**OP1-13 IECVA AND IPLS2-DA CLASSIFICATION TOOLS: A COMPARISON**

F. Savorani, Å. Rinnan, S.B. Engelsen

**OP1-14 MULTIVARIATE ANALYSIS APPLIED TO INDUSTRIAL PRODUCTION: TWO CASE STUDIES**

G. Polotti, R. Leardi

**OP1-15 USE OF FOURIER TRANSFORM-NEAR INFRARED SPECTRA TO DISCRIMINATE PATHOGENIC BACTERIA IN MILK**

F. Cámara-Martos, F. Pérez-Rodríguez, C.P. Coutinho, G. Zurera-Cosano, J.A.Lopes

**OP1-16 A MULTI-WAY APPROACH TO NEW WHEAT VARIETIES CHARACTERIZATION**

M. Li Vigni, C. Baschieri, A. Marchetti, G. Foca, A. Ulrici, M. Cocchi

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## **ORAL PRESENTATIONS: SESSION #2**

### **OP2-01 OLIVE OIL QUANTIFICATION IN VEGETABLE OIL BLENDS USING HPLC-CAD IN COMBINATION WITH CHEMOMETRIC TOOLS**

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

### **OP2-02 EXPLORATORY ANALYSIS OF HUMAN URINE BY LC-ESI-TOF MS AFTER HIGH INTAKE OF OLIVE OIL: UNDERSTANDING METABOLISM OF POLYPHENOLS**

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

### **OP2-03 VIRGIN OLIVE OILS QUALITY CONTROL BY CHEMOMETRIC TREATMENT OF RAMAN SPECTRA**

R. Korifi, Y. Le Dréau, J. Artaud, N. Dupuy

### **OP2-04 AUTHENTICATION OF ORGANIC OR NON ORGANIC HARD EWE CHEESES USING NEAR INFRARED SPECTROSCOPY**

M.I. González-Martín, J.M. Hernández-Hierro, I. Revilla, A. Vivar-Quintana, C. González-Pérez, L. Gómez García

### **OP2-05 FUSION OF METABOLOMICS AND PROTEOMICS DATA FOR BIOMARKERS DISCOVERY OF MULTIPLE SCLEROSIS**

L. Blanchet, A. Smolinska, A. Attali, T. Rosenling, M. Stoop, L. Coulier, M. Noga, S. Shi, A. Dane, K. Ampt, T. Tuinstra, T. Hankemeier, R. Bischoff, A. van Gool, S. Wijmenga, T. Luider, L. Buydens

### **OP2-06 CHEMOMETRIC APPROACHES FOR SCREENING AND PRIORITIZATION OF POPS, EDS AND PBTS BY QSAR**

E. Papa, P. Gramatica

### **OP2-07 CHEMOMETRIC-ASSISTED STUDY OF ATMOSPHERIC AND FLUVIAL POLLUTANT INPUTS IN THE GUADALQUIVIR RIVER ESTUARY**

J. A. López-López, M. García-Vargas, C. Moreno

### **OP2-08 <sup>1</sup>H-NMR AND UV-VISIBLE SPECTRA FUSION FOR DETERMINING SUDAN DYES IN CULINARY SPICES**

C. Di Anibal, I. Ruisanchez, M. P. Callao

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**OP2-09 MIXED LEVEL SUPERSATURATED DESIGN: CONSTRUCTION AND APPLICATION TO A GAS CHROMATOGRAPHIC METHOD FOR THE STUDY OF PEPPERMINT OIL**

M. Claeys-Bruno, C. Delaurent, R. Cela, R. Phan-Tan-Luu, M. Sergent

**OP2-10 COMPARISON OF BI AND TRI-DIMENSIONAL MULTIVARIATE METHODS IN ENVIRONMENTAL MONITORING**

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

**OP2-11 DETECTION OF PLASTIC FOREIGN BODIES IN FOOD APPLICATIONS WITH NIR HYPERSPECTRAL IMAGING**

L. Cervera, S. Fenollosa, C. Ávila, R. Díaz.

**OP2-12 ALTERNATIVE COMMON BASES FOR WAVELETS APPLICATION IN CHEMOMETRICS**

M. Forina, P. Oliveri, M. Casale

**OP2-13 ANÁLISE EXPLORATÓRIA APLICADA À AVALIAÇÃO DA COMPOSIÇÃO MINERAL DAS DUAS VARIEDADES DE REPOLHO COMERCIALIZADAS NO BRASIL**

D. Santos Anunciação, R. Mota de Jesus, S. L. Costa Ferreira