

# VII COLLOQUIUM CHEMIOMETRICUM MEDITERRANEUM

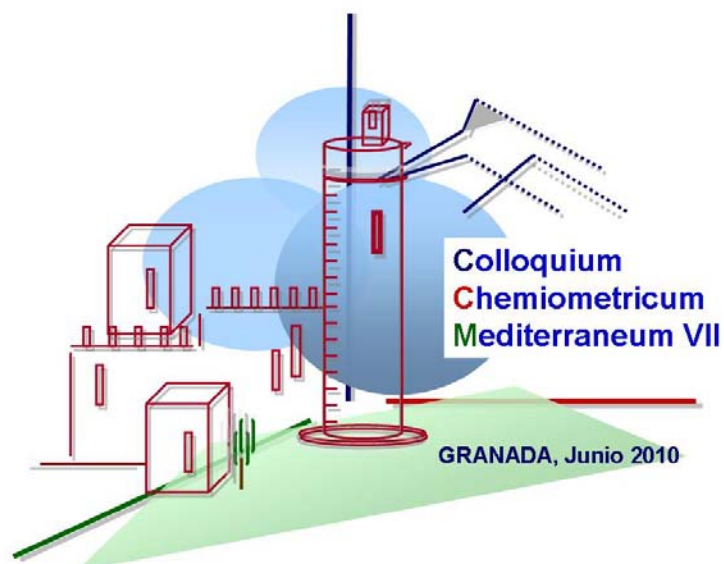


*CMM propinat opportunitatem exiniam  
ad intermutandum cognitiones a novitatibus collocatis  
in cuspide et rerum novarum*  
GRANADA, 21 - 24 JUNE 2010



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

## FULL PROGRAMME



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## MONDAY, 21th June

10:00 - 12:00 h : Registration

12:00 - 12:30 h : Inauguration. Rector of the University of Granada

12:30 - 13:15 h : Opening Lecture.

*L1 Forty years of chemometrics, forty years with chemometrics.  
Michele Forina*

**13:30 - 16:00 h : Lunch**

*(hang poster session 1)*

16:00 - 17:15 h : Oral session 1.1. Moderating: *Silvia Lanteri*

16:00 - 16:15 h :

*OP1-01* Optimisation of counter-propagation artificial neural networks by means of genetic algorithms.

*D. Ballabio, M. Vasighi, R. Todeschini.*

16:15 - 16:30 h :

*OP1-02* Application of missing data methods for exploratory data analysis in medical research.

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

16:30 - 16:45 h :

*OP1-03* Batch process using NIR spectroscopy in a quality by design approach.

*J. Rosas, M. Blanco, M. Alcalà.*

16:45 - 17:00 h :

*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.*

17:00 - 17:15 h :

*OP1-05* Fuzzy comparison of ballistic images.

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

**17:15 - 17:45 h : Coffee break**

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17:45 - 18:20 h : Invited lecture 1. *Moderating: Marcelo Blanco*  
*L2 Pitfalls and common mistakes in chemometrics.*  
*Rasmus Bro*

18:20 - 19:05 h : Oral session 1.2. *Moderating: Marcelo Blanco*

18:20 - 18:35 h :

*OP1-06 Multivariate Curve Resolution applied to the analysis of microarray data.*  
*J. Jaumot, B. Piña, R. Tauler.*

18:35 - 18:50 h :

*OP1-07 Bioreactor monitoring with spectroscopy and chemometrics: a review.*  
*N.D. Lourenço, J.A. Lopes, C.F. Almeida, M.C. Sarraguça and H.M. Pinheiro.*

18:50 - 19:05 h :

*OP1-08 Chemometric to investigate and resolve spectrokinetic data of ultrafast photoinduced processes.*  
*N. Mouton, B. Debus, M. Sliwa, A. De Juan, C. Ruckebusch.*

**19:30 -20:30 h : Guided Tour, "Hospital Real"**

**20:30 - 21:30 h : Reception UGR (at "Hospital Real")**

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## TUESDAY, 22th June

9:30 - 10:15 h : Oral session 1.3. Moderating: *Riccardo Leardi*

9:30 - 9:45 h :

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.*

9:45 - 10:00 h :

OP1-10 H value as analytical parameter in image analysis.

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

10:00 - 10.15 h :

OP1-11 Multidimensional non supervised analysis (textural and spatial) in MRI tomography for watercore detection.

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

10:15 - 10:50 h : Invited Lecture 2. Moderating: *Riccardo Leardi*

L3 Complex metabolomics data generates high-quality systems biology information

*Age Smilde*

### 10:50 - 11:10 h : Coffee Break

11:10 - 11:40 h : Poster session 1

*(simultaneously: CAMO presentation)*

11:40 - 12:15 h : Invited lecture 3. Moderating: *Magalie Claeys-Bruno*

L4 Tree-based classification methods for the interpretation of "omics".

*Max Feinberg*

12:15 - 12:45 h : Oral session 1.4. Moderating: *Magalie Claeys-Bruno*

12:15 - 12:30

OP1-12 Multivariate approach to data mining and data integration.

*L. Eriksson*

12:30 -12:45 h :

OP1-13 IECVA and IPLS2-da classification tools: a comparison.

*F. Savorani, Å. Rinnan, S.B. Engelsen.*

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## 12:45 - 12:50 h : Short break

12:50 - 13:35 h : Oral session 1.5. Moderating: M<sup>a</sup> Cruz Ortiz

12:50 - 13:05 h :

OP1-14 Multivariate Analysis Applied to Industrial Production: two case studies.

*G. Polotti, R. Leardi.*

13:05 - 13:20 h :

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.*

13:20 - 13:35 h :

OP1-16 A multi-way approach to new wheat varieties characterization.

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

## 13:40 - 16:00 h : Lunch

*(take down poster session 1 – hang poster session 2)*

16:00 - 17:15 h : Oral session 2.1. Moderating: Cyril Ruckebusch

16:00 - 16:15 h :

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.*

16:15 - 16:30 h :

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.*

16:30 - 16:45 h :

OP2-03 Virgin olive oils quality control by chemometric treatment of Raman spectra.

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

16:45 - 17:00 h :

OP2-04 Authentication of organic or non organic hard ewe cheeses using near infrared spectroscopy.

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

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17:00 - 17:15 h :

**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.*

**17:15 - 17:45 h : Coffee break**

17:45 - 18:20 h : Invited lecture 4. *Moderating: Marina Cocchi*

**L5** QSAR/QSPR: principles and fundamentals from a chemometric perspective.

*Roberto Todeschini.*

18:20 - 18:50 h : Oral session 2.2. *Moderating: Marina Cocchi*

18:20 - 18:35 h :

**OP2-06** Chemometric approaches for screening and prioritization of POPS, EDS and PBTS by QSAR.

*E. Papa, P. Gramatica.*

18:35 - 18:50 h :

**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*

**18:50 - 19:00 h : Short break**

19:00 h : General assembly SEQyC

**21:00 - 23:30 h : Flamenco dinner (at Peña "La Platería")**

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## WEDNESDAY, 23th June

9:30 - 10:15 h : Oral session 2.3. Moderating: M<sup>a</sup> Soledad Larrechi

9:30 - 9:45 h :

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.*

9:45 - 10:00 h :

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.*

10:00 - 10:15 h :

OP2-10 Comparison of bi and tri-dimensional multivariate methods in environmental monitoring.

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

10:15 - 10:50 h : Invited lecture 5. Moderating: M<sup>a</sup> Soledad Larrechi

*L5 Plans d'expériences: quand la réponse est fonctionnelle (Designs of experiments: the treatment of functional responses)*

*Michelle Sergent*

**10:50 - 11:10 h : Coffee break**

11:10 - 11:40 h : Poster session 2

*(simultaneously: Umetrics presentation)*

11:40 - 12:15 h : Invited lecture 6. Moderating: Rafael Cela

*L6 Chemometrics for residue testing.*

*Luis Sarabia*

12:15 - 13:00 h : Oral session 2.4. Moderating: Rafael Cela

12:15 - 12:30 h :

OP2-11 Detection of plastic foreign bodies in food applications with NIR hyperspectral imaging.

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

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12:30 - 12:45 h :

OP2-12 Alternative common bases for wavelets application in chemometrics.

*M. Forina, P. Oliveri, M. Casale.*

12:45 - 13:00 h :

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.*

**13:00 - 13:05 h : Short break**

13:05 - 13:40 h : Invited lecture 7. *Moderating: Rafael Cela*

*L7 Use of multivariate resolution results for hyperspectral image interpretation.*

*Anna de Juan*

**13:45 - 16:00 h : Lunch**

*(take down poster session 2)*

**16:00 - 21:00 h : Guided tour**

Route 1: Visit to "Alpujarra"

Route 2: Visit to Granada coast

**21:30 - 00:30 h : Congress dinner (at Salobreña, Granada Coast)**



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## THURSDAY, 24th June

10:00 - 10:15 h : Awards ceremony

**10:15 - 10:35 h : Coffee break**

**10:35 - 12:30 h : TRIBUTE to Prof. Michele Forina**

Speakers: *Luis Sarabia, Consuelo Pizarro, Roger Phan-Tan-Luu, Michele Forina.*

Recital: Choir of the Faculty of Educational Sciences, University of Granada

12:45 - 13:00 h : Closing ceremony

13:00 - 14:00 h : Farewell cocktail