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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

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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

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

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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

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

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

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

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

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

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

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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

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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

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

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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

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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

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F. Marini, B. Walczak

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R. Tauler, J. Jaumot.

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

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

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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

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

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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

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

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J.L. Villa, J. Ferré, R. Boqué

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

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

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M. Hernández Revilla, M. Vega Alegre

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

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

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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

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

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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

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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

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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

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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

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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

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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

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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.

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

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

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ad intermutandum cognitiones a novitatibus collocatis
in cuspide et rerum novarum*
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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

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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

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