

POSTER SESSION 1- Monday (30/06/2008) and Tuesday (01/07/2008)

Advances in chemometrics

- S1-01 A normalized youden-plot in interlaboratory proficiency tests
de la Mata-Espinosa, Aídee Paulina; Cuadros-Rodríguez, Luis; Bosque-Sendra, Juan Manuel; Ruiz Samblás, Cristina
- S1-02 Acceptance areas in SIMCA method
Pomerantsev, Alexey L.
- S1-03 Line width issues with generalized 2D correlation NMR spectroscopy
Kirwan, Gemma; Adams, Mike
- S1-04 Sulfur determination in vacuum and atmospheric residue of petroleum using ATR-FTIR-PLS
Muller, Edson Irineu; Parisotto, Graciele; Hermes, Aline Lima; Santos, Maria de Fátima Pereira dos; Guimarães, Regina Célia Lourenço; Dressler, Valderi Luiz; Flores, Erico Marlon de Moraes
- S1-05 Evaluation of evidence value of glass fragments by likelihood ratio and Bayesian Network approaches
Zadora, Grzegorz
- S1-06 Simultaneous determination of acetylsalicylic acid, paracetamol and caffeine using solid-phase molecular fluorescence and PARAFAC
Alves, Júlio César L.; Poppi, Ronei Jesus
- S1-07 PARAFAC2 for classification of weathered diesel oils: a bridge between ASTM and nordtest methods
Ebrahimi Mohammadi, Diako; Brynn Hibbert, David
- S1-08 No-alignment-strategies for the analysis of two-dimensional chromatographic signals
Daszykowski, Michal; Danielsson, Rolf; Walczak, Beata
- S1-09 Robust modeling of the antioxidant capacity of green tea based on chromatographic fingerprints
Daszykowski, Michal; Vander Heyden, Yvan; Walczak, Beata
- S1-10 Dealing with missing elements and outliers in PCA, SIMCA and PLS
Stanimirova, Ivana; Walczak, Beata
- S1-11 Second-order advantage when applying different artificial neural networks after unfolded principal component analysis/residual bilinearization
Goicoechea, Héctor C.; García-Reiriz, Alejandro; Damiani, Patricia; Culzoni, Maria Julia; Olivieri, Alejandro C.
- S1-12 The use of net analyte signal (NAS) in NIR spectroscopy: interpretability and figures of merit.
Sarraguça, Mafalda Cruz; Lopes, João Almeida

- S1-13 Shelf-life determination using NIR spectroscopy and the multivariate accelerated shelf-life test
Pedro, André Krell; Ferreira, Márcia Miguel Castro
- S1-14 Concentration profiles determination for chemical reactions using standard Multivariate Curve Resolution-Alternating Least Square (MCR-ALS) and hard-modeling.
Naef, Olivier; Daul, Claude
- S1-15 Analysis of adulteration in argan oil using infrared spectroscopy and chemometrics
Oussama, Abdelkhalek; Devos, Olivier
- S1-16 A new approach to estimate the numbers of factors in residual bilinearization for BLLS and UPLS models
Braga, Jez Willian Batista; Carneiro, Renato Lajarim; Poppi, Ronei Jesus
- S1-17 Classifying NIR spectra of textile products with different supervised pattern recognition methods
Durand, Alexandra; Devos, Olivier; Ruckebusch, Cyril; Huvenne, Jean-Pierre; Vander Heyden, Yvan
- S1-18 Wavelet transform-based clustering of spectra in chemometrics
Ukil, Abhisek; Bernasconi, Jakob; Braendle, Hubert
- S1-19 Simultaneous variable and sample selection for PLS calibrations using a robust genetic algorithm
Comas, Enric; Wiegand, Pat; Pell, Randy
- S1-20 Comparison of different pretreatment methods to FTIR infrared spectra of grape must and their influence in the goodness of PLS fit
Cervera, Lorenzo; Díaz, Ricardo; Carot, Jose Miguel
- S1-21 Evaluation of chemometric methods for the investigation of environmental pollution sources
Terrado, Marta; Barceló, Damià; Tauler, Romà
- S1-22 Fourier and wavelet coefficients filtering for near infrared instrument calibration and standardization
Igne, Benoit; Hurburgh, Charles R.
- S1-23 Estimation of uncertainty in PLS models using the Principal Components Transform (PCT) approach
Barros, António de Sousa; Rutledge, Douglas N.
- S1-24 Characterization of gas engine oils by IR and chemometrics
Felkel, J.; Dörr, N.; Leimeter, T.; Novotny-Farkas, F.; Varmuza, K.
- S1-25 A study on using chemometrics for the integration of acoustic and chemical data: Early detection of fires in confined spaces
Statheropoulos, M.; Mikedi, K.; Pallis, G. C.; Stavrakakis, P.

- S1-26 A new strategy for calibration transfer of MLR models based on the successive projections algorithm (SPA)
Pereira, Claudete Fernandes; Pimentel, Maria Fernanda; Galvão, Roberto Kawakami Harrop; Honorato, Fernanda Araújo; Stragevitch, Luiz
- S1-27 A classification tool for N-way array based on SIMCA methodology
Cocchi, Marina; Durante, Caterina; Bro, Rasmus
- S1-28 Determination of glucose and ethanol in bioethanol production by near-infrared spectroscopy and chemometrics
Liebmann, Bettina; Friedl, Anton; Varmuza, Kurt
- S1-29 Leave-n-samples-out cross-validation in PCA for missing data recovery and robustness in front of measurement noise
Camacho, José; Picó, Jesús; Ferrer, Alberto
- S1-30 Double regularization for temperature correction with Tikhonov regularization. Application to calibration transfer
Goicoechea, Héctor C.; Siano, Gabriel G.; Andries, Erik; Kalivas, John H.
- S1-31 Detection limit estimator for multivariate calibration
Ostra, Miren; Ubide, Carlos; Vidal, Maider; Zuriarrain, Juan
- S1-32 Detecting periodicity in online NIR data
Paakkunainen, Maaret; Kohonen, Jarno; Reinikainen, Satu-Pia
- S1-33 Non linear class-modeling
Marini, Federico; Magri, Antonio L.; Bucci, Remo; Magri, Andrea D.
- S1-34 Backward Variable Selection PLS (BVSPLS)
Fernandez, Juan Antonio; Baeten, Vincent; Dardenne, Pierre
- S1-35 Comprehensive description of the kinetic pathway and species involved in the photodegradation of decabromodiphenyl ether (DecaBDE) using chromatographic, spectroscopic and chemometrics tools
Mas, Sílvia; de Juan, Anna; Lacorte, Sílvia; Tauler, Romà
- S1-36 Chemometrics tools for monitoring master tasters performance in the evaluation of Aceto Balsamico Tradizionale di Modena (ABTM)
Durante, Caterina; Cocchi, Marina; Grandi, Margherita; Marchetti, Andrea; Amorotti, Vincenzo Ferrari
- S1-37 Non-linear PLS approach in score surface
Kohonen, Jarno; Reinikainen, Satu-Pia; Höskuldsson, Agnar
- S1-38 Understanding the molecular bases of cathodic stripping voltammetry: a novel QSPR strategy
Giussani, Barbara; Monticelli, Damiano; Todeschini, Roberto; Dossi, Carlo

- S1-39 Combination of chemometric advances for discriminating biological samples based on their GC-MS analysis. Application to food authentication
Engel, Erwan; Ratel, Jérémy; Lehallier, Benoist; Bakkali, Asmae
- S1-40 Using non-linear methods for NIR prediction of ingredient composition of intact animal feeds
Fernandez-Ahumada, Elvira; Garrido, Ana; Gómez, Augusto; Guerrero, Jose Emilio; Perez-Marin, Dolores; Vallesquino, Pedro; Sanchez, Lourdes; Diaz, Esperanza; Fearn, Tom
- S1-41 Prediction of λ_{\max} of 1,4-naphthoquinone derivatives using ant colony optimization
Atabati, Morteza; Zarei, Kobra; Mohsennia, Mahbobeh
- S1-42 Building a regression vector for variable selection
Ferreira, Márcia M. C.; Teófilo, Reinaldo F.
- S1-43 Preliminary study on use NIR spectroscopy for the determination of bruise damage and storage time in mushrooms
Esquerre, Carlos; Gowen, Aoife; O'Donnell, Colm; Downey, Gerard
- S1-44 MDL wavelet denoising of coaveraged NIR spectra
José, Gledson Emidio; Galvão, Roberto Kawakami Harrop; Araújo, Mário César Ugulino
- S1-45 Signal processing in chromatography
Pap, Tamas L.
- S1-46 Chemometrics approach for simultaneous optimization of resolution, time of analysis and ruggedness of separation in MLC
Boichenko, Alexander; Kulikov, A.U.; Galater.kharkov.ua, M.N.; Yakovleva, E.Yu.; Loginova, L.P.
- S1-47 PLS-trees in data mining and clustering
Eriksson, Lennart; Trygg, Johan; Wold, Svante
- S1-48 O2PLSTM for improved analysis and visualization of complex data
Eriksson, Lennart; Wold, Svante; Trygg, Johan
- S1-49 Reactive Spectrometers
Brown, Christopher David; Green, Robert L.
- S1-50 Qualitative interpretation of regression vectors: part II
Brown, Christopher David; Green, Robert L.
- S1-51 ORWEBILR a practical computer code for fitting linear calibration curves with replicated measurements using bivariate, weighted and ordinary least-squares regression models
Santoyo, E.; Díaz-González, L.

POSTER SESSION 1- Monday (30/06/2008) and Tuesday (01/07/2008)

Process analysis

- S1-52 Use of MCR-ALS in the study of jojoba oil ageing by IRTF
Nathalie, Dupuy; Muriel, Makewetche; Yveline, Le Dreau; J., Joachim; Jacky, Kister
- S1-53 Monitoring of a fluid-bed-drying and a film-coating process
Lutz, Holger; Schleimer, Michael; Niemöller, Andreas
- S1-54 Multivariate modeling of reactionkinetics - the hydrosilylation of styrene and triethylsilane
Imlinger, Nicolas Christian; Blattner, Christian; Krell, Manfred; Schmeer, Georg
- S1-55 Application of near infrared spectroscopy and multivariate control charts for B2(biodiesel/diesel) monitoring
Oliveira, Ingrid Komorizono; Rocha, Wéricson Fortunato; Poppi, Ronei Jesus
- S1-56 High temperature gas chromatography applied to characterization of crude oils: a chemometric approach
Dias, Julio César Magalhães; Tamanqueira, Juliana Boechat; Camacho, Cristina Fourquet
Bandeira; Vicente, Maristela de Araujo; de Castro, Eustáquio Vinicius Ribeiro; de Medeiros, Edna Faria; de Aguiar, Paula Fernandes
- S1-57 Rank analysis of spectral reaction data for factor-analytical methods
Amrhein, Michael; Bhatt, Nirav; Bonvin, Dominique
- S1-58 Estimation of compatibility of drug and starch acetate to form a sustainable matrix tablet
Matero, Sanni Elina; Reinikainen, Satu-Pia; Lahtela-Kakkonen, Maija; Hakulinen, Mikko; Ketolainen, Jarkko; Poso, Antti
- S1-59 Quality control of packed raw materials in pharmaceutical industry
Rodionova, Oxana; Sokovikov, Yaroslav; Pomerantsev, Alexey
- S1-60 Multivariate Analysis for quality control of blends in oil exploration and production: a study case
Sad, Cristina Maria dos Santos; Filgueiras, Paulo Roberto; Vicente, Maristela de Araujo; de Medeiros, Edna Faria; de Castro, Eustáquio Vinicius Ribeiro; Dias, Julio César Magalhães
- S1-61 The reliable PAT strategy: Achieving on-line measurement robustness
Chauchard, Fabien; Roussel, Sylvie; Fontange, Cécile
- S1-62 Figures of merit for determination of alcohol content in cachaça by short-wave near-infrared spectroscopy
Althmann Maretto, Danilo; Fortunato de Carvalho Rocha, Werickson; Poppi, Ronei Jesus
- S1-63 Using robust MSPC methods to improve on the quality of animal feed
Verboven, Sabine; Goos, Peter; Hubert, Mia

- S1-64 At-line control of an industrial bread-making process
Li Vigni, Mario; Brettagna, Barbara; Cocchi, Marina; De Marco, Tommaso; Foca, Giorgia; Marchetti, Andrea; Ulrici, Alessandro
- S1-65 Fermentation reaction characterisation using multiple-scattered light in the NIR region
Dzhongova, Elitsa Zdravkova; Harwood, Colin R.; Thennadil, Suresh N.
- S1-66 Representative sampling and weighbridge NIR characterization of grape juice - Implementing Process Analytical Technologies (PAT) in the winemaking process
Esbensen, Kim Harry; Swanepoel, Marinda
- S1-67 Comparison of NIR and fluorescence spectroscopy techniques for the real time characterization of crude oil
Le Roux, Galo Carrillo; Sotelo, Francisco Falla; Nascimento, Claudio Oller; Quina, Frank Herbert; Pantoja, Patricia Araujo; Gejo, Juan Lopez; Camolesi, Valmir Jose; Katata, Antonio Carlos
- S1-68 Application of spectroscopic techniques and chemometric tools to study the chemical evolution of vegetable oils during heating
Estephan, Nathalie; Ouaini, Naim; Locquet, Nathalie; Rutledge, Douglas
- S1-69 Simple chemometrics methods and the discovery of a new chemical phenomenon: The system methanol-ethanol
Mello, Cesar; Noda, Isao; Ricci, Emiliane; Sevéri, Eza; Marangoni, Antônio; Coelho, Lucinda; Ribeiro, Diórginis; Poppi, Ronei
- S1-70 Measuring biodecolorization of textile wastewater with a multivariate approach
Lourenço, Nídia Dana; Coelho, Marta Isabel; Pinheiro, Helena Maria
- S1-71 Characterization of wastewater treatment plant sludges for agricultural use by NIR spectroscopy
Paixão, F.; Akyüz, F.; Lourenço, N. D.; Pinheiro, H. M.
- S1-72 Possible optimization of drinking-water disinfection processes for controlling the formation of disinfection by-products by linear and non-linear modelling
Platikanov, Stefan; Tauler, Romà
- S1-73 Enabling PAT with the lighthouse probe
Bogomolov, Andrey; Melichar, Michael; Wigmore, A.; Grau, Kathrin
- S1-74 Towards the spectrophotometric monitoring of aromatic amines in textile effluent treatment
Almeida, Cláudio Fernandes; Lourenço, Nídia Dana; Pinheiro, Helena Maria
- S1-75 Which calibrate function could I get best results with?
Veiga, Jose Manuel; Cabonell, Vicente; Moreno, Amelia
- S1-76 Chemometrics on a PDA
Cauchi, Michael

- S1-77 Robustness of accuracy profile for method validation: application to food microbiological control
Feinberg, Max; Boubetra, Abdelkader
- S1-78 Study of a model reaction for obtaining thermosets from vegetable oils using NIR spectroscopy and Multivariate Curve Resolution – Alternating Least Squares
del Río Sánchez, Vanessa; Pilar Callao, M.; Soledad Larrechi, M.; Montero de Espinosa, Lucas; Carles Ronda, J.; Cádiz, Virginia
- S1-79 Quantitative resolution of FTIR-ATR spectra obtained in the monitoring of cationic curing of DGEBA and g- valerolactone using multivariate curve resolution method (MCR-ALS)
Spegazzini, Nicolas; Ruisánchez, Itziar; Larrechi, M. Soledad; Serra, Angels; Mantecón, Ana
- S1-80 Implementation of NIR analysers for in-line monitoring of drying processes
Despagne, Frederic
- S1-81 Methods of calibrating NIRS sensors when biological parameters are correlated: the case of maize amino acids
Hardy, Connie L.; Rippke, Glen R.; R. Hurburgh. Jr., Charles; Goldstein, Walter A.
- S1-82 Decision rules based on the estimate of a proportion of measurements
Bertrand, Frédéric; Maumy, M.
- S1-83 Moisture content determination of pharmaceutical pellets by near-infrared spectroscopy: model selection, evaluation and validation
Mantanus, Jérôme; Ziémons, E.; Lebrun, P.; Rozet, E.; Klinkenberg, R.; Streel, B.; Hubert, Ph.
- S1-84 Multivariate statistical process control using the MSPCA software. Application to the monitoring of the simulated wastewater treatment plant performance
González-Martínez, José María; Ferrer, A.
- S1-85 Batch Processing of Spectra using Distributing Computing
Kussener, Florence

POSTER SESSION 2- Wednesday, Thursday and Friday (02/07/2008-04/07/2008)

Chemo- & bio-informatics

- S2-01 Early experience in the NIR-based detection of counterfeit drugs
Rodionova, Oxana; Pomerantsev, Alexey
- S2-02 On line photochemically induced excitation-emission-kinetic four-way data. Analytical application for the determination of folic acid and its two main metabolites in serum by N-PLS/Residual Trilinearization (RTL) calibration
Muñoz de la Peña, Arsenio; Jiménez Girón, Ana; Durán-Merás, Isabel; Espinosa, Anunciación; Olivieri, Alejandro C.
- S2-03 Studying the solution equilibria of G-quadruplex region upstream of the B-cell lymphoma-2 P1 by means of multivariate data analysis methods
del Toro, Miquel; Jaumot, Joaquim; Aviñó, Anna; Eritja, Ramon; Gargallo, Raimundo
- S2-04 Quantification of adulterants in gasoline by GC x GC and N-PLS
de Godoy Jr., Luiz Antonio Fonseca; Ferreira, Ernesto Correa; Pedroso, Marcio Pozzobon; Augusto, Fabio; Poppi, Ronei Jesus
- S2-05 Classification of DNA structures by means of chemometrical methods
Jaumot, Joaquim; del Toro, Miquel; Gargallo, Raimundo; Eritja, Ramon
- S2-06 Determination of significant compounds related to bitterness and “grain taste” in volatile profile of beers through GA variable selection
da Silva, Gilmore Antonia; Maretto, Danilo Althmann; Bolini, Helena Maria André; Augusto, Fabio; Poppi, Ronei Jesus
- S2-07 Quantitative structure relationships for volatile organic compounds using semi-empirical topological index (IET)
Heinzen, Vilma Edite Fonseca; Junkes, Berenice Da Silva; Yunes, Rosendo Augusto; Souza, Erica Silva
- S2-08 Simultaneous kinetic-potentiometric determination of aluminum(III) and zirconium (IV) using H-point standard addition method and partial least squares
Karimi, Mohammad Ali
- S2-09 Simultaneous kinetic-potentiometric determination of hydrogen peroxide and peroxyacetic acid using H-point standard addition method and chemometric methods
Karimi, Mohammad Ali
- S2-10 Quantification of propranolol enantiomers by partial least squares regression and near-infrared spectroscopy
Valderrama, Patrícia; Poppi, Ronei Jesus
- S2-11 Quantification of biodiesel by using fourier-transform near-infrared spectroscopy and multivariate calibration
Oliveira, Ingrid Komorizono; Rocha, Wéricson Fortunato; Poppi, Ronei Jesus

- S2-12 Direct determination of ibuprofen enantiomers in urine by spectrofluorimetry with the aid of second order advantage
Valderrama, Patrícia; Poppi, Ronei Jesus
- S2-13 Exploration of linear multivariate calibration techniques to predict the total antioxidant capacity of green tea from chromatographic fingerprints
Dumarey, Melanie; van Nederkassel, Anne-Marie; Deconinck, Eric; Vander Heyden, Yvan
- S2-14 Genetic algorithm and NPLS for determination of riboflavin and pyridoxine on milk preparations by molecular fluorescence
Carneiro, Renato Lajarim; Braga, Jez Willian Batista; Poppi, Ronei Jesus
- S2-15 Application of hard modeling as a chemometrics method for kinetic study of promethazine-orthophenantroline-Fe(III) reaction
Tavallali, Hossein; Golshan, Azadeh
- S2-16 Kinetic spectrophotometric study of oxidation of paracetamol by Fe(III) with non-linear least square regression
Tavallali, Hossein; Golshan, Azadeh
- S2-17 Mild-heating effects on the molecular structure of milk components as investigated by synchronous front-face fluorescence spectroscopy coupled with parallel factors (PARAFAC) analysis
Dufour, Eric; Boubellouta, Tahar
- S2-18 Interval PLS_Cluster: Investigation of different criteria indicating the quality of the clustering
Jouan-Rimbaud Bouveresse, Delphine; Rutledge, Douglas N.
- S2-19 Comparative study of partial least squares and orthogonal signal correction-partial least squares for the simultaneous determination of ceratine, creatinine, and uric acid
Khajehsharifi, Habibollah; Sadeghi, Masoomeh
- S2-20 Multivariate calibration applied to a highly interfering chemical system the simultaneous spectrophotometric determination of hydroquinone and catechol in real sample
Khajehsharifi, Habibollah; Sadeghi, Masoomeh
- S2-21 Evaluation of nitrogen oxide variation patterns in Catalonia during the period from 2001 to 2006 using multivariate data analysis methods
Alier, Marta; Felipe-Sotelo, Monica; Hernandez, Isabel; Tauler, Roma
- S2-22 Calculation of spectra and equilibrium concentration profiles by matrix method
Kudrev, Andrei
- S2-23 Annual changes of chemical and physical properties in the Ross Sea surface waters (Antarctica)
Massolo, Serena; Messa, Roberta; Rivaro, Paola; Leardi, Riccardo

- S2-24 Chemometrics for early diagnosis of peritonitis in PD patients
Bloemberg, Tom G.; Pluk, W.; Gloerich, J.; Wehrens, R.; van den Heuvel, L.P.; Buydens, L.M.C.
- S2-25 Multiway PCA and MCR investigation of the effect of pH and UV radiation on kinetic degradation of anthocyanin mixtures extracted from flower dyes
Março, Paulo Henrique; Tauler, Romà; Poppi, Ronei Jesus
- S2-26 Comparison of methods for selection of chromatographic columns
Heberger, Karoly; Kalivas, John H.
- S2-27 Prediction of unit cell parameters of ABX3 perovskites using counter-propagation neural networks
Aleksavska, Slobotka; Dimitrovska Lazova, Sandra; Kuzmanovski, Igor; Novič, Marjana
- S2-28 Estimating the compactness of peptide dendrimers using counter-propagation neural networks
Kuzmanovski, Igor; Javor, Sacha Javor; Reymond, Jean-Louis; Novič, Marjana
- S2-29 Error back-propagation neural network as a mapping device towards food specifications
Novič, Marjana; Grošelj, Neva
- S2-30 Exploratory analysis of structural properties of DNA-intercalator complexes in crystalline state
Ferreira, Márcia M. C.; Kiralj, Rudolf
- S2-31 3-Way pattern-recognition of PAHs from Galician seawater samples after the Prestige's wreck (2002-2005)
Fernandez-Varela, Raquel; Grueiro-Noche, Gloria; Andrade, Jose Manuel; Muniategui, Soledad; Lopez-Mahia, Purificación; Prada, Dario
- S2-32 3-Way pattern-recognition of soils by procrustes rotation, matrix-augmented principal components analysis and parallel factor analysis
Fernandez-Varela, Raquel; Andrade, Jose Manuel; Kubista, Mikael; Carlosena, Alatzne; Prada, Dario
- S2-33 Using fluorescence spectroscopy and multiway methods to monitor the electrochemical oxidation of phenolic compounds on boron-doped diamond electrode
Ferreira, Márcia M. C.; Teófilo, Reinaldo F.; Peterlevitz, Alfredo C.; Ceragioli, Helder J.; Bro, Rasmus; Barauskas, Vitor; Kubota, Lauro
- S2-34 Drift compensation of gas sensor array data by orthogonal signal correction
Padilla, Marta; Perera, Alexandre; Montoliu, Ivan; Chaudry, A.; Persaud, Krishna; Marco, Santiago
- S2-35 using multivariate curve resolution with rank augmentation and feasibility constraints to monitor beef cooking in situ with ATR/FTIR spectroscopy
Smith, Sean; Elmore, Doug; Muroski, Allen

- S2-36 Data fusion strategies for nutrimentomics
Peré-Trepat, Emma; Montoliu, Ivan; Martin, François-Pierre; Rezzi, Serge; Kochhar, Sunil
- S2-37 Multivariate and multiway analyses of 2D-chromatogram obtained by “Comprehensive GCxGC”: study of the effectiveness of the prior alignment of the chromatograms
Noçairi, Hicham; Rutledge, Douglas N.
- S2-38 OPLS and dynamic modeling in clinical metabolomics
Stendlund, H; Calderisi, M; Madsen, R; Tassini, M; Valensin, G; Carmellini, M; Lundstedt, T; Vivi, A; Trygg, J
- S2-39 Disease diagnosis in metabolomics
Madsen, Rasmus; Moritz, Thomas; Ekström, Gunilla; Lundstedt, Torbjörn; Trygg, Johan
- S2-40 Pattern Recognition methods to classify spilled oils and medium-heavy distillates according to their contents on PAHs
Fernandez-Varela, Raquel; Andrade, Jose Manuel; Grueiro-Noche, Gloria; Muniategui, Soledad; Prada, Dario; Ramírez-Villalobos, Francisco; Vazquez-Campo, Javier
- S2-41 Principal Component Transform for PLS2 (PCT-PLS2)
Jouan-Rimbaud Bouveresse, Delphine; Rutledge, Douglas N
- S2-42 A chemometric study of HPLC chromatograms of extracts from different teas
Zheng, Liang; Watson, Dave; Johnston, Blair; Edrada-Ebel, RuAn
- S2-43 Quantitative monitoring of photo-degradation process of three dyes from tanning effluents applying MCR-ALS to the UV-visible spectra obtained using a SIA methodology
Fernández Barrat, Cristina; Pilar Callao, Maria; Soledad Larrechi, Maria
- S2-44 Classification of Sudan dyes by means of rapid methodologies based on spectroscopy techniques and chemometric approach
Di Anibal, Carolina Vanesa; Pilar Callao, M.; Ruisánchez, Itziar
- S2-45 The molecular descriptor log SumAA and its alternatives in QSRR models to predict the retention of peptides
Bodzioch, Karolina; Bączek, T.; Vander Heyden, Y.; Kaliszan, R.

POSTER SESSION 2- Wednesday, Thursday and Friday (02/07/2008-04/07/2008)

Experimental design

- S2-46 Multilevel data analysis of a crossover designed human nutritional study
Velzen, E.J.J. van; Westerhuis, J.A.; Duynhoven, J.P.M. van; Dorsten, F.A. van; Hoefsloot, H.; Draijer, R.; Kroner, C.I.; Smit, S.; Smilde, A.K.
- S2-47 Application of multivariate optimization in the development of an ultrasound-assisted extraction procedure for multielemental determination in bean samples using ICP OES
Korn, Maria das Graças Andrade; Santos, Wagna Piler Carvalho dos; Castro, Jacira Teixeira; Bezerra, Marcos de Almeida; Fernandes, Andréa Pires; Ferreira, Sérgio Luis Costa
- S2-48 Variance analysis of nicotine and nicotine free dry particulate matter in fine-cut smoking articles
Heberger, Karoly; Kephelopoulos, S.; Kemeny, S.; Dymond, H.; Wilkes, E. B.; Kotzias, D.
- S2-49 Optimization of method for the determination of iron in petroleum condensate by ETAAS
Ferreira, Sergio LC; Fernandes, Marcelo S; Rebouças, Marcio V; Korn, Maria GA; Santos, Walter NL
- S2-50 Box-Behnken design in the optimization of a preconcentration procedure for copper determination from river waters
Bezerra, Marcos Almeida; Moreno, Islania; Santos, Queila Oliveira; Santos, Walter Nei Lopes; Barros, Joélia Martins
- S2-51 Box-Behnken design in the Optimization of an on-line pre-concentration system for determination of lead by TS-FF-AAS
Ferreira, Hadla Sousa; Matos, Geraldo D; Ferreira, Sergio Luis Costa
- S2-52 Mixed level supersaturated designs: a useful tool for the determination of the robustness of a gas chromatographic method
Clayeyes-Bruno, Magalie; Delaurent, C.; Cela, R.; Sergent, M.
- S2-53 Central composite design with/without artificial neural networks in microemulsion LC separation robustness testing
Jancic Stojanovic, Biljana Savo; Malenovic, A.; Ivanovic, D.; Medenica, M.
- S2-54 Chromatographic separation of a pharmaceutical formulation using Design of Experiment and Design Space
Debrus, Benjamin; Lebrun, P.; Ceccato, A.; Caliaro, G.; Rozet, E.; Rupérez, J.; Barbas, C.; Boulanger, B.; Hubert, Ph.

POSTER SESSION 2- Wednesday, Thursday and Friday (02/07/2008-04/07/2008)

Image analysis

- S2-55 Pattern matching algorithms for comprehensive gas chromatography
Adams, Mike; Marriott, Philip
- S2-56 Hyperspectral near infrared imaging for biological/chemical studies of organic material (biltong): standardisation, pre-processing and chemometrics for exploration and classification
Manley, Marena; Williams, Paul; Geladi, Paul
- S2-57 Dynamic skin characterisation using multivariate target factor analysis and FTIR spectroscopy
Mader, K.; Mitchell, J.; Chan, K.L.A.; Kazarian, S.G.; Tetteh, J.
- S2-58 Partial least squares regression for prediction of mushroom (*Agaricus bisporus*) slice quality during storage
Gowen, Aoife Ann
- S2-59 Particle detection in near-infrared images by image segmentation using mathematical morphology
Gendrin, Christelle; Roggo, Yves; Collet, Christophe
- S2-60 Spectroscopic imaging below the diffraction limit: myth or reality?
Duponchel, Ludovic; Milanfar, Peyman; Ruckebusch, Cyril; Huvenne, Jean-Pierre
- S2-61 Multivariate image analysis: state of the art
Prats-Montalbán, José Manuel; Ferrer, Alberto
- S2-62 Sourcing counterfeit tablets using NIR-CI - a case study
Lopes, Marta; Wolff, Jean-Claude
- S2-63 Correlation between sludge settleability and image analysis information using Partial Least Squares
Mesquita, Daniela P.; Dias, Oscar; Dias, Ana M. A.; Amaral, António L.; Ferreira, Eugénio C.
- S2-64 Hybrid network flow for peak-tracking in multi-dimensional NMR experiments
Ravel, Patrice; Guilhem, Kister; Marc André, Delsuc
- S2-65 Using Angle Measure Technique as a feature extractor for analysis of non-isotropic images
Kucheryavskiy, Sergey; Belyaev, I.