Colloquium Spectroscopicum Internationale XLII

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BOOK OF ABSTRACTS

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GELP Grupo de ESPECTROSCOPÍA LÁSERES Y PLASMAS

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POSTER SESSION THURDAY, JUNE 2nd / FRIDAY, JUNE 3rd

PO-TF-01	***Juan Miguel Gil de la Fe***	*Spectroscopic diagnostics of laboratory astrophysics experiments on radiative shocks launched in xenon using helium as a tracer*
PO-TF-02	***María Luisa Carvalho***	*Quantification of trace elements in eco-innovative biofortified farmed fish by means of a polarized geometry, secondary target XRF spectrometer*
PO-TF-03	***Lorena Placer Vidal***	*Citric acid/cysteamine luminescent probe for bromine speciation using a smartphone-based fluorimetric sensing*
PO-TF-04	***Vanesa Romero Rivas***	*Ultrasound-assisted dispersive (micro)solid phase extraction of synthetic fragrances using a covalent organic framework as adsorbent followed by fluorescent determination*
PO-TF-05	***Paula Rodríguez Rodríguez***	*Synthesis and physicochemical characterization of zirconium oxide nanoparticles using a simple hydroxide precipitation methodology.*
PO-TF-06	***Mª Luisa Cervera Sanz***	*Acrylamide determination in homemade toasts using smartphone digital colorimetry*
PO-TF-07	***Hooriyeh Borhani***	*Nondestructive Determination of Tomato Qualitative Parameters Using Raman Spectroscopy*
PO-TF-08	***Barbara Štádlerová***	*Comparison of radiation sources for atomic fluorescence spectrometry*
PO-TF-09	***Vanessa Antunes***	*Spectroscopic multianalytical techniques to illustrate Zurbarán Spanish influence in Óbidos, Portugal, painting workshop*
PO-TF-10	***Claudia Masucci***	*Spectroscopic Lights and Shadows of Direct Air Capture*
PO-TF-11	***Carlos Alberto Lopes Antunes***	*Discrimination of different monovarietal wines by FTIR-ATR*
PO-TF-12	***Mario Menéndez Miranda***	*Evaluation of NIRS technology for honey quality control analysis*
PO-TF-13	***Sumusu Imashuku***	*X-Ray-excited optical luminescence imaging for rare-earth-elements bearing minerals*
PO-TF-14	***Flavio Nakadi***	*Study of the possibilities of high-resolution molecular absorption using a continuous source in a graphite furnace for the measurement of different Sr isotopes*
PO-TF-15	***Franz Hallwirth***	*Development and characterization of a novel microwave assisted, high-pressure, flow digestion system for subsequent elemental analysis*
PO-TF-16	***Rafael Rodríguez Pérez***	*MIXKIP/RAPCAL: a 2D atomic kinetics and radiative transfer computational package for spectroscopic diagnostics of high energy density plasmas*
PO-TF-17	***Margarida Nunes***	*An exploratory study on the blotting materials used in the Portuguese monastic scriptoria during the Early Modern period*
PO-TF-18	***Alexander A Kamnev***	*An original set of vibrational coordinates for 2D calculation of the tunneling splittings due to inversion motion of H_3O^+*
PO-TF-19	***David Vicente Zurdo***	*Neuroprotective activity of selenium nanoparticles against the effect of amino acid enantiomers in Alzheimer's disease*
PO-TF-20	***Jasna Jablan***	*Critical evaluation of the use of dispersive Raman spectroscopy for quantification of active pharmaceutical ingredients (API) in pharmaceutical formulations*
PO-TF-21	***Felix Weigand***	*Characterization of a Mobile Solution Cathode Glow Discharge Optical Emission Spectrometry Instrument*
PO-TF-22	***Cristina Gonzalez Gago***	*New prospects of Glow Discharge Mass Spectrometry towards depth profiling of ultrathin layers*

PO-TF-11.-Discrimination of different monovarietal wines by FTIR-ATR

Carlos Antunes [1]*, Cláudia Carrilho[2], Fátima Peres[1,3], Rodolfo Queirós[2], Cecília Gouveia[1], Cristina Canavarro[1], António Ramos[1], Ofélia Anjos[1,4]

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Abstract

Wine is a strategic sector in the beverages industry and is constantly linked to changes in consumption and an increase in their quality. However, if the most popular monovarietal wines are well characterized some minor or regional varieties don't have until now a complete characterization. In the last years, many researches were developed applying vibrational spectroscopy methodologies for food and beverages industry and in particular for wine industry, as an easy way to predict wine properties or to distinguish between groups of samples. Concerning that, the aim of this research was characterize some Portuguese varieties of wine monovarietal wines and distinguish them by Fourier Transform Infrared Spectroscopic method with Attenuated Total Reflectance (FTIR-ATR).

Red and white wines from different grape varieties were used in this study. The red wines were produced with 'Aragonês' (syn. 'Tinta Roriz'), 'Touriga Nacional', 'Touriga Franca', 'Rufete' and some blends of those varieties. White wines were produced with 'Arinto', 'Síria' and several wine blends. The analytical parameters acetic acid, alcohol, citric acid, density, fructose, glucose, glycerol, lactic acid, malic acid, pH, saccharose, tartaric acid, total acidity and total sugars were measured by FTIR-ATR using commercial calibration. Spectra were acquired with a FTIR (Bruker spectrometer, Alpha) equipped with a diamond single reflection attenuated total reflectance (ATR). Four spectra per sample were obtained, in the range of 4000 to 450 cm^{-1}, with 128 scans per spectrum at a spectral resolution of 8 cm^{-1} according to the methodology previously described [1]. The device is equipped with a flow-through cell with controlled temperature and the background was measured with distilled water. Chemometric analyses of spectral information were performed using the Unscrambler® X, version: 10.5.46461.632 (CAMO Software AS, Oslo, Norway) and OPUS®, version: 7.5.18 (Bruker Optic, Germany).

The more relevant spectral regions to differentiate the wines was situated at 3000 to 2800 cm^{-1}; 1400 to 1200 cm^{-1} and 1000 to 800 cm^{-1}. The results, for both red and white monovarietal wines, showed different chemical characteristics, allowing to distinguish them with chemometric techniques. With principal component analysis (PCA) made with spectral data, it is also possible to discriminate between wines produced with different varieties. However, some multivarietal wines showed similar composition of the monovarietal ones and, consequently, were more difficult to distinguish with the multivariate analysis. The results showed a good potential of FTIR-ATR, with chemometric analysis, to discriminate monovarietal red and white wines.

Keywords: FTIR-ATR; Wine; Chromatography; Grape varieties; Chemometrics.

References

[1] R. Sánchez-Gómez, O. Anjos, I. Nevares, T. Delgado, M. Del Alamo-Sanza. Vitis 58 (Special Issue), (2019) 77–82

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