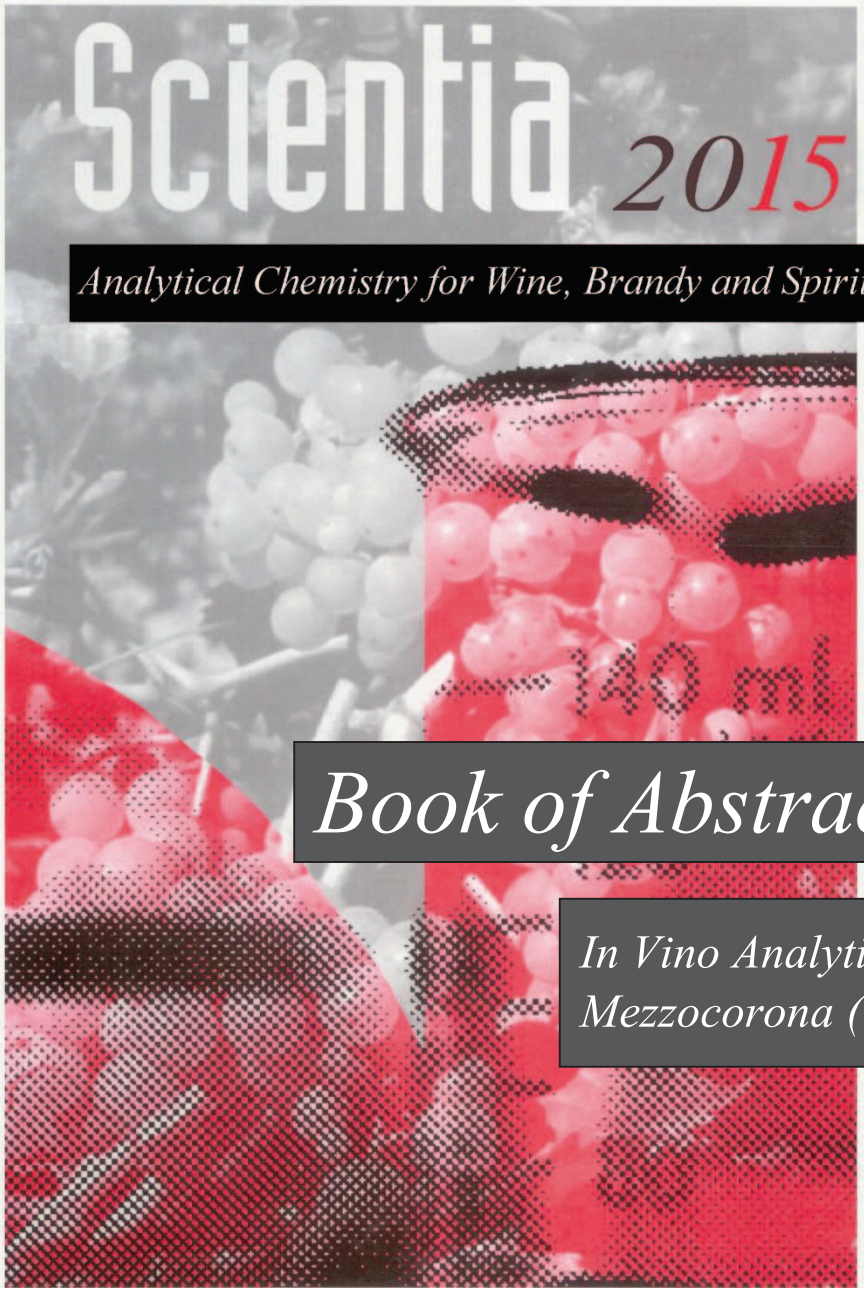
NINTH SYMPOSIUM

In Vino Analytica Scientia 2015

Analytical Chemistry for Wine, Brandy and Spirits



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In the method development, the adaptations focused on maintaining the ionic strength of the eluents constant and using an hybrid quadrupole-time of flight HRMS detector. This allowed to simplify the sample preparation and study the effectiveness of LC-HRMS for long batches, in order to record the maximum number of metabolites with good chromatographic resolution and the best MS stability and accuracy. Results from the wine storage experiment showed that slightly sub-optimum storage temperature had a major impact on the polar metabolite fingerprint of red wines, with a clear trend of deterioration along the time points.

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REFERENCE

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CHEMAN Y21 - Establishing an atmospheric pressure gas chromatography-MS (APGC-MS) based metabolomics platform

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ABSTRACT - Metabolomics has become a powerful tool to study biological processes in organisms and to identify metabolites and Gas chromatography coupled with mass spectrometry (GCMS) is a well-established analytical approach in metabolomics. The most widely used ionization technique in GCMS is electron ionization (EI), which produces library searchable spectra dominated by fragments. The molecular ion in EI spectrum is often of very low abundance or absent. Many plant terpenoids have same molecular formula and shows matching fragmentation pattern when using EI, therefore any minor variation in the relative abundances of the masses in a spectrum lead to a false positive hit in NIST. Also lack of molecular ion information can give incorrect compound identification, if using spectral matching alone. Alternative approaches, such as the chemical ionization (CI), can be optimized to provide a molecular ion with reduced fragmentation, but with the serious drawback of a major loss of the sensitivity. Atmospheric pressure gas chromatography coupled with mass spectrometry (APGC-MS) is an ionization technique that generates a spectrum conserving the molecular ion species with minimal fragmentation; additionally the system offers high mass accuracy, which is extremely useful in structure elucidation of unknown volatiles. We are establishing Atmospheric Pressure Gas Chromatography-MS (APGC-MS) Based Metabolomics Platform for volatile plant metabolites; primary results using Grape as a model sample are presented.