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Application Summary Compendium

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Application Summary AN 20853

Determination of Catechins and Phenolic Acids in Red Wine by Solid Phase Extraction and HPLC

Monica Dolci, Thermo Fisher Scientific, Runcorn, Cheshire, UK

Overview:

The catechin group of flavanols are major components in wine and are reported to have antioxidant, antimicrobial, antimutagenic and anticarcinogenic activities and polyphenols contribute to the taste, appearance, and formation of unappetizing flavors.

This application note shows a fast and efficient sample preparation and gradient HPLC method for determination of catechins and other polyphenols in red wine.

Method:

A solid phase extraction (SPE) procedure was established using Thermo Scientific™ HyperSep™ Retain PEP SPE cartridges. Separation was performed using a Thermo Scientific™ Accucore™ PFP 2.6µm 100 x 2.1mm HPLC column on a Thermo Scientific™ Accela™ UHPLC system.

Part Number	Description
60107-204	HyperSep Retain PEP 200mg 3mL
17426-102130	Accucore PFP 2.6µm 100 x 2.1mm

Conclusion:

An HPLC method for the analysis and quantitation of nine catechins and phenolic acids from red wine was developed. Extraction of these polar analytes was achieved on HyperSep Retain PEP material, and shows excellent recovery. The unique selectivity offered by the Accucore PFP HPLC column provides exceptional separation performance to resolve these very structurally similar compounds.

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AB72110-EN 0816M-W1

Application Summary AN 20830

Determination of 24 Pesticide Residues in Red Wine Using a QuEChERS Sample Preparation Approach and LC-MS/MS Detection

Mike Oliver, Thermo Fisher Scientific, Runcorn, UK

Overview:

The analysis of pesticide residues in red wine is challenging due to the complexity of the matrix, which contains alcohol, organic acids, sugars, and polyphenols.

Sample preparation involves the extraction of pesticides from red wine using the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) extraction method. The samples then undergo cleanup by dispersive solid-phase extraction (dSPE) using primary secondary amine (PSA) sorbent, which effectively retains organic acids, sugars, and phenolic pigments.

Method:

A modified QuEChERS (AOAC version), extraction method was used along with dispersive solid-phase extraction (dSPE). The purified extract was separated using the Thermo Scientific™ Accucore™ aQ 2.6µm 100 x 2.1mm HPLC column and Thermo Scientific™ Accucore™ aQ Defender™ 2.6µm 10 x 2.1mm guard column to facilitate fast and high efficiency separations on a Thermo Scientific™ Dionex™ UltiMate™ 3000 LC system. Detection was carried out on a Thermo Scientific™ TSQ Vantage™ tandem mass spectrometer in ESI+ mode. Data processing was carried out using Thermo Scientific™ TraceFinder™ software.

Part Number	Description
60105-335	Mylar Pouch with 6g $MgSO_4$ and 1.5g Sodium Acetate
60105-350	2mL Centrifuge Tube with 150mg $MgSO_4$ and 150mg PSA
17326-102130	Accucore aQ 2.6µm 100 x 2.1mm
17326-012105	Accucore aQ Defender Guard 10 x 2.1mm

Conclusion:

A fast, easy and cost-effective method has been successfully developed using the QuEChERS-based approach. The Accucore aQ HPLC columns gave good resolution and peak shapes for all of the pesticides. Good linearity, low LOQs, and satisfactory accuracy and precision data were obtained, indicating that this method is suitable for pesticide residue analysis in red wine.

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AB72110-EN 0816M-W2

Isotope Analysis of Water, Fruit Juice and Wine Using the Thermo Scientific GasBench II IRMS

Andreas W. Hilkert, Hairigh Avak
Thermo Fisher Scientific, Bremen, Germany

Overview:

The measurement of the $^{18}O/^{16}O$ ratio of water is one of the most important applications of isotope ratio mass spectrometry. Authenticity control of wine demand a general purpose analytical solution which can provide high precision, high accuracy and high throughput analysis. ^{18}O isotopic analysis of wine has been a topic of increasing interest, and is now the subject of EU regulation and other countries.

Method:

The Thermo Scientific™ GasBench II Isotope Ratio Mass Spectrometer (IRMS) was used. Samples of wine were run on both the GasBench II and the HDO II water equilibrator in a comparison study. The wine samples were analyzed directly, without distillation.

Conclusion:

Successful analysis of natural waters, fruit juices, and wines shows that the GasBench II IRMS can be used for isotope studies on a wide range of water-bearing substrates. Measuring a suite of natural waters which included a much depleted antarctic water establishes that the GasBench II IRMS has no memory, and that there is no cross talk between samples as is so often the case for water preparation devices.

Read the full application note

AB72110-EN 0816M-W3

Application Summary AN 30147

^{13}C and Simultaneous ^{18}O and ^{2}H Isotope Analysis in Ethanol with Thermo Scientific DELTA V Isotope Ratio Mass Spectrometers

Oliver Kracht, Andreas Hilkert, Thermo Fisher Scientific, Bremen, Germany;
Tünde Racz-Fazakas, Chemical Institute of the Hungarian Customs and Finance Guard, Budapest, Hungary

Overview:

Isotopic analyses of wine has become a widespread tool to evaluate the quality, authenticity and origin. This application note shows the ability and performance of the analysis of ethanol with combustion and with a high temperature carbon reduction technique in combination with a gas Isotope Ratio Mass Spectrometer (IRMS).

Method:

The elemental analyser used was a Thermo Scientific™ FlashEA1112 HT with a single reactor system combining combustion and reduction in one reactor. Detection using a Thermo Scientific™ DELTA V™ Isotope Ratio Mass Spectrometer (IRMS).

Conclusion:

C isotopes of ethanol can be measured easily and with low cost using standard equipment and tin capsules for liquids. Precision is better than 0.1%. H and O isotopes of ethanol can be measured simultaneously with high precision and with a high throughput of up to 200 samples/day.

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Application Summary AN 30173

Direct Analysis of Red Wine Using Ultra-Fast Chromatography and High Resolution Mass Spectrometry

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Frantisek Pehal, NNH Hospital Na Homolce, Prague, Czech Republic
Martin Hornshaw, Thermo Fisher Scientific, Hemel Hempstead, UK

Overview:

Red wine is a very complex mixture and a rich source of beneficial anti-oxidants. Identification and quantitation of these natural products is challenging. Ultra High Pressure Liquid Chromatography (UHPLC) coupled to a mass spectrometer enables simultaneous detection and relative quantitation of wine's antioxidant constituents and progressive changes after exposure to air. This application note demonstrates the feasibility of analyzing complex mixtures without any prior sample preparation by making use of the high resolving power of both UHPLC and the Orbitrap mass analyzer detector.

Method:

Chromatography of wine samples was performed using a Thermo Scientific™ Accela™ UHPLC with a Thermo Scientific™ Hypersil GOLD™ 1.9µm 100 x 2.1mm column. Detection was carried out using a Thermo Scientific™ LTQ Orbitrap XL™ mass spectrometer, with Thermo Scientific™ SIEVE™ 1.2 software.

Part Number	Description
25002-102130	Hypersil GOLD 1.9µm 100 x 2.1mm

Conclusion:

UHPLC affords fast analysis times while maintaining very high chromatographic resolution (peak width 7 seconds at half height). Accurate mass measurements significantly improves the precision of quantitation by eliminating nearly all isobaric interferences. This is a particularly important aspect for complex mixture analyses such as red wine.

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AB72110-EN 0816M-W5

Iron, Copper and Zinc Determination in Wine using Flame Atomic Absorption Spectroscopy

Dr Anastasia Gadzhieva, AA Applications Chemist, Thermo Fisher Scientific, Cambridge, UK

Overview:

Some metals can affect the quality of the wine, in particular zinc, copper and iron, which can lead to haze formation in bottled wine. It is therefore recommended that winemakers screen for these metals prior to bottling. In addition, due to the increased use of copper sulfate as a fining agent, copper levels in wine are rising worldwide. It is essential to ensure that levels are below the maximum recommended of 0.5 mg/L for copper and 30 mg/L for iron and zinc that is stipulated by EU directive EC 606/2009. The prescribed method of analysis is Flame Atomic Absorption Spectroscopy (FAAS).

Method:

A Thermo Scientific™ iCE™ 3300 AA was used for the FAAS measurements of iron, copper and zinc in different wine samples. The Thermo Scientific™ SOLAAR™ software contains pre-set spectrometer parameters for iron, copper and zinc and these were used to measure the samples.

Conclusion:

The iCE 3300 AA demonstrates an ideal solution for iron, copper and zinc determination in wine samples following dilution. The optimization wizards within the Thermo Scientific SOLAAR software make method development simple and ensure optimum analytical conditions.

Read the full application note

AB72110-EN 0816M-W6

Application Summary AN 43355

Analysis of Trace Elements and Major Components in Wine with the Thermo Scientific iCAP 7400 ICP-OES

Sanja Asendorf, Application Specialist, Bremen, Germany

Overview:

The natural level of trace elements in wine is typically nontoxic. Agricultural practice however can change the composition of the trace element budget of the vineyard, for example of Hg, Pb, Sn, and Zn. Elements such as Cu, Mn, and Zn are increased due to use of fertilizers and pesticides. In addition, the acidity of wine and must (freshly pressed grape juice) can dissolve Cr, Cu, Ni, and Zn from wine making equipment like pumps and taps. Due to these processes the concentration of heavy metals like As, Cd, Hg and Pb can rise and reach toxic levels. Therefore, the quality of the wine has to be determined not only for nutritional reasons but also for consumer safety.

Method:

For the sample analysis, the Thermo Scientific™ iCAP™ 7400 ICP-OES Duo was used together with an aqueous sample introduction kit. A Teledyne CETAC ASX-560 autosampler was used to transfer the sample to the introduction system of the ICP-OES. The Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) software was used for data acquisition.

Conclusion:

The analysis shows that the Thermo Scientific iCAP 7000 Plus Series ICP-OES delivers excellent accuracy and sensitivity for determination of nutrients and trace elements in wines in conformity with the present recommendations for concentration limits. The powerful software platform Qtegra ISDS simplifies method development and makes post-processing of the sample data an easy operation.

Read the full application note

AB72110-EN 0816M-W7

Application Summary AN 52242

Identification and Quantification of Impurities in Wines by GC-MS

Benedicte Gauriat-Desroy, Eric Phillips, Stacy Crain, Trisa Robarge
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(With special thanks to members of Oenologic Center of Grezillac)

Overview:

Wine makers have historically used gas chromatography and mass spectrometry, (GC-MS) to detect pesticides, they now more commonly use the technique to supplement quality control checks of wine taste. Without GC-MS, wine makers must rely on expert evaluation by oenologists to determine wine quality. By identifying maturation tracers and molecules commonly responsible for taste defects, GC-MS augments expert opinion with objective and quantitative information. The method described in this application note allows wine makers to obtain precise measurements on the organoleptic parameters that determine wine purity on site, rather than having to send samples for expensive, external analysis.

Method:

Samples were prepared using a SPME (solid-phase microextraction) PDMS/DVB 65µm StableFlex™ SPME Fiber. An ISQ mass spectrometer was used to perform sequential full scan/SIM acquisitions. A Thermo Scientific™ TRACE™ GC Ultra™ with a Thermo Scientific™ TraceGOLD™ TG-5MS 15 m × 0.25 mm × 0.25 µm column was used. Results were analyzed using Thermo Scientific™ QuanLab™ Forms software. QuanLab Forms is also Directorate-General for Health and Consumer Protection (SANCO) compliant and can be used in the European Union.

Part Number	Description
26098-1300	TraceGOLD TG-5MS 15m x 0.25mm x 0.25µm

Conclusion:

The ability of the ISQ GC-MS to detect several contaminants in wine at lower concentrations than the limit of human tasters, and its ease of use in combination with a single-step, two-minute sample preparation, make it a useful tool for the wine industry. This general method may be customized to particular wines by incorporating new parameters such as trying other SPME coatings in the extraction phase.

Read the full application note

AB72110-EN 0816M-W8

Fast and Accurate Automated Method for Free Sulfite Analysis in Wine

Eric Naigeon,[1] Marco Rastetter,[2] Mari Klemm,[3] and Annu Suoniemi-Kähärä3
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[3]Thermo Fisher Scientific, Vantaa, Finland

Overview:

Sulfur dioxide (SO_2) is added to control the process of wine making. The presence of total SO_2, both free and bound, is regulated and, as a result, a warning statement is required on wine labels because sulfite, is considered an allergen. The European Union established a maximum permitted level of total SO_2 in wine of 500 mg/L, in the USA, the maximum level of total SO_2 permitted is 350 mg/L.

An automated method to measure free SO_2 in wine samples is presented.

Method:

The method is based on the reaction between sulfur dioxide, *p*-rosaniline hydrochloride, and formaldehyde. This method is designed to use optimal reagent concentrations and volumes to provide accurate results.

A Thermo Scientific™ Gallery™ discrete photometric analyzer was used for this study. The SO_2 Free system reagents kit for Gallery analyzers were used.

Conclusion:

The automated photometric Thermo Scientific SO_2 Free method correlates well with the FIA method. This new automated SO_2 Free method is very quick and easy to use. Analysis of 60 samples takes only 35 min and allows simultaneous analysis of various sugars and acids, color, and total SO_2. Compared to the FIA method, the photometric method requires only small volumes of reagents, thus being the more economically and environmentally friendly choice. This method enables a laboratory to fully automate SO_2 determinations and replace traditional time consuming reference and distillation methods.

Read the full application note

AB72110-EN 0816M-W9

Application Summary AN 71653

An Enzymatic Method for Acetaldehyde Testing of Alcoholic Beverages

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[1]University of Helsinki, Department of Food and Environmental Sciences, Division of Food Chemistry, Helsinki, Finland
[2]Thermo Fisher Scientific, Vantaa, Finland, [3]Alko Inc., ACL, Helsinki, Finland

Overview:

Acetaldehyde (ethanal, CH_3CHO) is found in alcoholic beverages and many other foods, like yogurts, that are produced by fermentation processes. Yeasts and bacteria produce acetaldehyde as their metabolites. It is also naturally present in fruits like apples. Acetaldehyde is produced when the human body breaks down ethanol. Aldehyde dehydrogenase (ALDH2) is the major enzyme responsible for oxidizing acetaldehyde into acetic acid. In 2009, the International Agency for Research on Cancer (IARC) concluded that consuming acetaldehyde with alcohol is carcinogenic to humans.

The objective of this study is to develop and validate a rapid enzymatic method based on photometric UV determination for acetaldehyde and compare it with a liquid chromatographic method.

Method:

A Thermo Scientific™ Arena™ 20XT analyzer was used for the automated photometric determination. The Thermo Scientific Gallery™ and Gallery™ Plus analyzers can also be used for this test. The Thermo Scientific Acetaldehyde system kit was used for enzymatic analysis of acetaldehyde.

20 Samples were analyzed during the method validation phase including wine, spirits, beer, and cider.

Conclusion:

The enzymatic method correlated very well with the liquid chromatography method as shown in this study. Enzymatic determination of acetaldehyde provides a rapid, user-friendly way of analyzing acetaldehyde from alcoholic beverages.

Read the full application note

AB72110-EN 0816M-W10

A Comparison Study of Total Acidity Methods for the Analysis of Wine

Sari Hartikainen, Mari Kiviluoma, Leena Kaski, and Annu Suoniemi-Kähärä
Thermo Fisher Scientific, Vantaa, Finland

Overview:

In Europe, total acidity in musts and wines is defined by the Office International de la Vigne et du Vin (OIV), whereas in the US, the Association of Official Analytical Chemists (AOAC), has established alternative parameters.

Often there is confusion with terminology, because titratable acidity (TA) and total acidity are often used interchangeably. Total acid content is defined as the concentration of organic acids in grapes and wine whereas TA is a measure of the hydrogen ions consumed by titration.

Wine samples measured with the Thermo Scientific™ Total Acids method are compared in this study to results from the traditional titration method.

Method:

The Thermo Scientific™ Gallery™ analyzer was used for automated photometric determination. A Thermo Scientific Total Acids (Wine, pH 7) system kit was used for colorimetric analysis of total acidity. Samples were run without pre-treatment or pre-dilution steps.

Conclusion:

The automated colorimetric method can be used for all the sample types tested because the colorimetric method correlated very well with the titration method.

Along with the Total Acids method, other colorimetric or enzymatic methods, such as glucose, fructose, acetaldehyde, total polyphenol, calcium and sulphur dioxide can be run simultaneously on the analyzer.

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Application Summary AN 71838

Evaluation of a Fully Automated Method for the Measurement of Glycerol in Wine

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[2]Alcohol Control Laboratory, Alko Inc., Helsinki, Finland

Overview:

During fermentation, glycerol is synthesized from the glucose within yeast cells. Glycerol is the third most common chemical compound in wines and an important by-product of alcoholic fermentation. The influence of glycerol in finished wine is usually at or below the level of sensory perception. Wines with elevated levels of alcohol tend to have more body and viscosity and a sweet taste which has often been attributed to the presence of glycerol.

Method:

The Thermo Scientific™ system reagent kit for determination of glycerol in wine was used. Results were obtained using a Thermo Scientific™ Arena™ 20XT analyzer and a WineScan FT120 (FOSS). The Glycerol method has also been adapted for use with the fully automated discrete Thermo Scientific Gallery™ and Gallery™ Plus analyzers.

Conclusion:

The Thermo Scientific Glycerol test used with the Arena discrete analyzer is accurate and repeatable both at high and low levels. The results correlate well with those measured by the WineScan™ and also with those analyzed according to the accredited ALKO, Inc. enzymatic method.

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