Table of Contents

Chromatography for Profiling Beverages

Applications Notebook

Methods for Composition Analysis

Thermo SCIENTIFIC

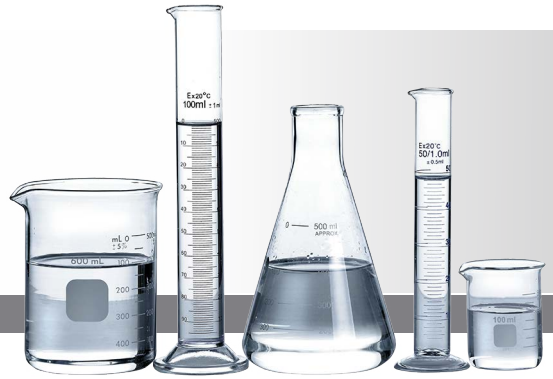
Table of Contents

Profiling Beverages

Introduction

Beverages are potable liquids specifically prepared for human consumption and include both non-alcoholic (tea, coffee, milk, juices, soft drinks, and carbonated drinks) and alcoholic (wine, beer, spirits) drinks. This section examines the measurement of the different compounds found in a variety of beverages.

Table of Contents



Analytical Technologies

High-Performance Liquid Chromatography

Thermo Scientific™ Vanquish™ UHPLC System and Thermo Scientific™ Dionex™ UltiMate™ 3000 UHPLC+ systems offer excellent chromatographic performance, operational simplicity and unrivaled flexibility. Choose from a wide range of standard and unique specialty detectors to extend your laboratory's analytical capabilities.

Thermo SCIENTIFIC

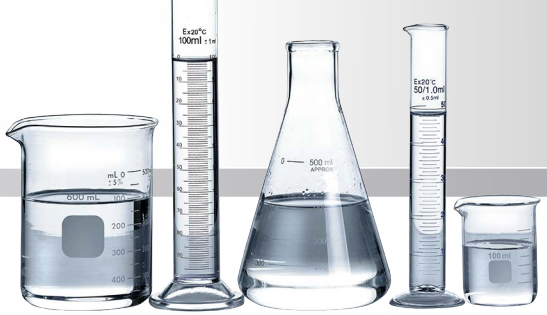


Table of Contents

The Vanquish UHPLC System

The next generation in UHPLC innovations

The Vanquish system takes high-end UHPLC to a new level, offering more resolution while meeting the throughput demands of modern laboratories. The system is delivers better separations, more results and easier interaction, simultaneously, without compromise.

Delivering the new standard in UHPLC

- More powerful separations with 1500 bar of pump pressure at flow rates up to 5 mL/min
- Industry-leading flow and gradient precision
- Excellent injections up to 100 µL in 0.01 µL increments
- Automated workflows with barcode reading for simplified setup and tracking
- Maximum sample capacity with up to 23 well plates, or 8832 samples
- More confident separations with a wide temperature range of 5 °C to 120 °C for two thermostatting modes and active column pre-heating for improved precision
- UV detection with linear response up to 3000 mAu and noise levels as low as 3 µAu
- Thermo Scientific™ LightPipe™ technology assures lowest peak dispersion with UV detection
- Available Vanquish Charged Aerosol detector for quantification of non-chromophoric compounds

Vanquish Diode Array Detector with LighPipe technology

Thermo SCIENTIFIC

Learn more at www.thermoscientific.com/vanquish

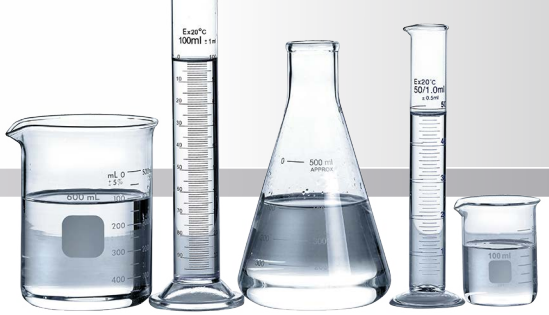
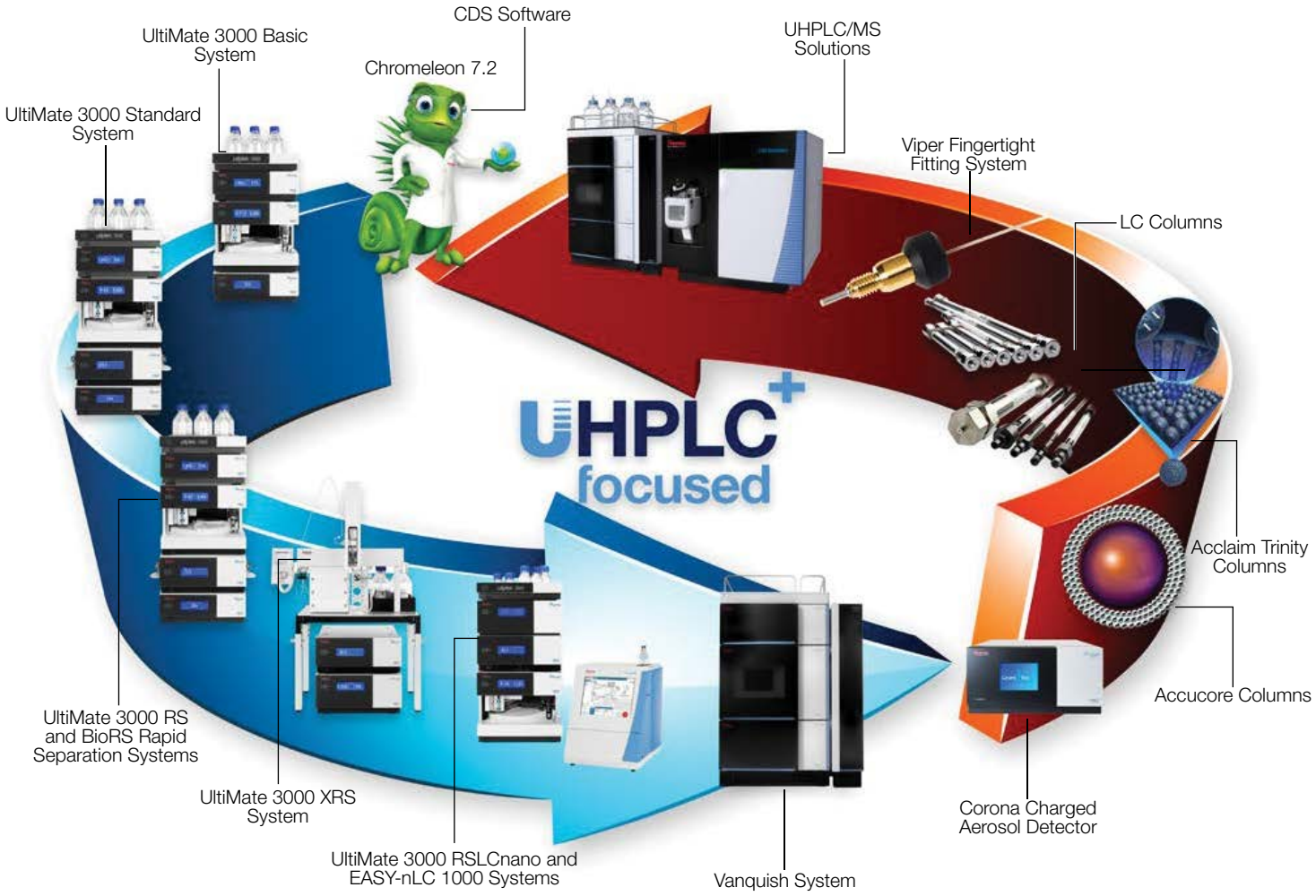
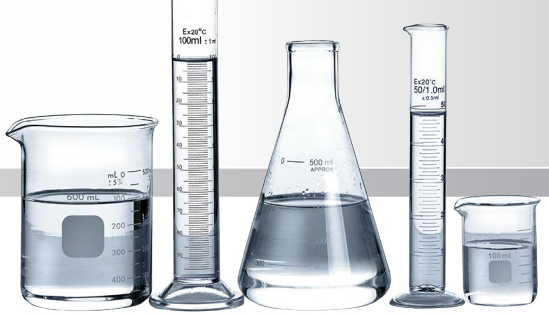


Table of Contents

UHPLC Portfolio



Thermo SCIENTIFIC



UltiMate 3000 UHPLC+ Systems

Best-in-class HPLC systems for all your chromatography needs

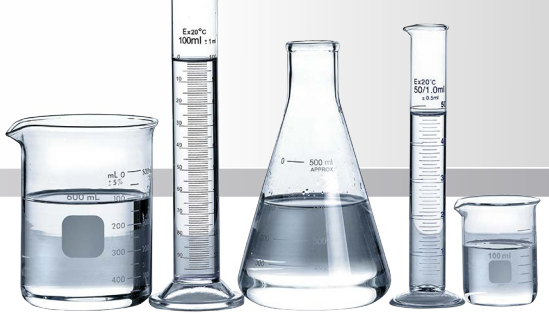
UltiMate 3000 UHPLC+ Systems provide excellent chromatographic performance while maintaining easy, reliable operation. The basic and standard analytical systems offer ultra HPLC (UHPLC) compatibility across all modules, ensuring maximum performance for all users and all laboratories.

Covering flow rates from 20 nL/min to 10 mL/min with an industry-leading range of pumping, sampling, and detection modules, UltiMate 3000 UHPLC+ Systems provide solutions from nano to semipreparative, from conventional LC to UHPLC.

Superior chromatographic performance

- UHPLC design philosophy throughout nano, standard analytical, and rapid separation liquid chromotography (RSLC)
- 620 bar (9,000 psi) and 100 Hz data rate set a new benchmark for basic and standard analytical systems
- RSLC systems go up to 1000 bar and data rates up to 200 Hz
- ×2 Dual System for increased productivity solutions in routine analysis
- Fully UHPLC compatible advanced chromatographic techniques
- Thermo Scientific™ Dionex™ Viper™ and nanoViper™ fingertight fittings—the first truly universal, fingertight fitting system even at UHPLC pressures

Table of Contents



UltiMate 3000 UHPLC+ Systems

We are uniquely focused on making UHPLC technology available to all users, all laboratories, and for all analytes.

Table of Contents

Rapid Separation LC Systems
The extended flowpressure footprint of the RSLC system provides the performance for ultrafast high-resolution and conventional LC applications.

Standard LC Systems
Choose from a wide variety of standard LC systems for demanding LC applications at nano, capillary, micro, analytical, and semipreparative flow rates.

RSLCnano Systems
The Rapid Separation nano LC System (RSLCnano) provides the power for high resolution and fast chromatography in nano, capillary, and micro LC.

Basic LC Systems
UltiMate 3000 Basic LC Systems are UHPLC compatible and provide reliable, high performance solutions to fit your bench space and your budget.

Thermo SCIENTIFIC

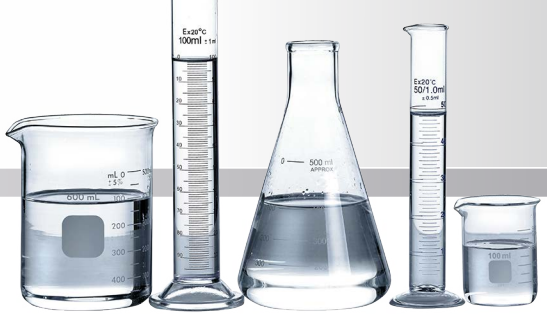


Table of Contents

Advanced Detection Capabilities

Charged Aerosol Detection

Charged Aerosol Detection provides near universal detection independent of chemical structure for non- or semi-volatile analytes with HPLC and UHPLC. Thermo Scientific™ Dionex™ Corona™ Veo™ and Vanquish Charged Aerosol detectors are ideally suited as a primary detector for any laboratory, while providing complementary data to UV or MS methods. No other LC detector available today can match the performance of a Corona Veo detector.

- High sensitivity – single-digit nanogram on column
- Consistent response – independent of chemical structure
- Wide dynamic range – to four orders of magnitude or greater
- Simple to use – easy to integrate with any HPLC/UHPLC system

Charged aerosol detectors give the simplicity, reproducibility and performance required for a full range of applications from basic research to manufacturing QC/QA. With charged aerosol detection you get predictable responses to measure analytes in direct proportion to their relative amounts for quantitation without actual standards.

This detector offers the flexibility to use reversed-phase gradients, as well as normal phase and HILIC modes of separation on any LC system. And, in many cases eliminates the need for derivatization or sample pre-treatment to provide real dilute-and-shoot simplicity.

Corona Veo Charged Aerosol Detector

Vanquish system with Charged Aerosol Detector

Thermo SCIENTIFIC

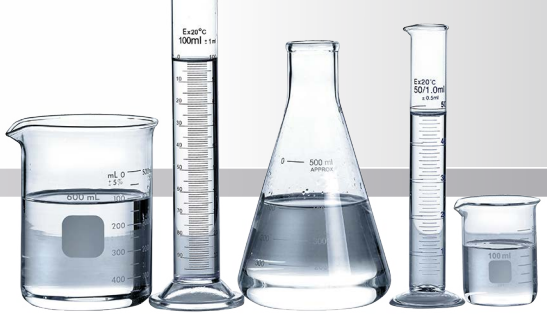


Table of Contents

Advanced Detection Capabilities

CoulArray Multi-electrode Array Detector

The Thermo Scientific™ Dionex™ CoulArray™ Multi-electrode Array detector is the only practical multi-channel electrochemical detection system that allows you to measure multiple analytes simultaneously, including those that are chromatographically unresolved. The CoulArray detector delivers the widest dynamic range of any available electrochemical detector with unmatched selectivity for detection of trace components in complex matrixes, even when used with aggressive gradients.

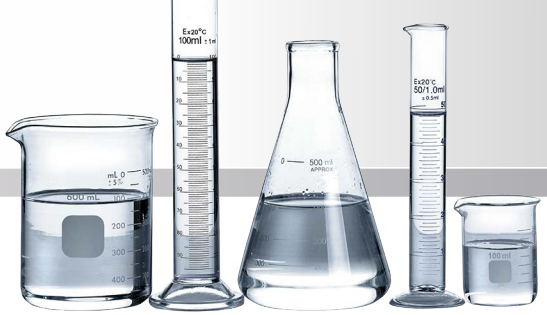
- Measures analytes from femtomole to micromole levels
- Greatly simplify sample preparation and eliminate interferences
- Simultaneously analyze multiple analytes in very complex samples
- Easily produce qualitative information for compound identification

Multiple system configurations offer 4, 8, 12, or 16 channels that can be upgraded anytime. The unique data acquisition and processing software uses automatic signal ranging and a unique patented baseline correction algorithms to provide identification and quantitation of single or multiple analytes and powerful 3D data for quick sample fingerprint confirmation with integration to pattern recognition platforms.

With the power of coulometric array technology, the CoulArray detector can give you the qualitative data of a optical PDA with 1,000 fold greater sensitivity to profile the characteristic qualities of products, determine integrity, identify adulteration and even evaluate competitors' products.

CoulArray Multi-electrode Array Detector

Thermo SCIENTIFIC



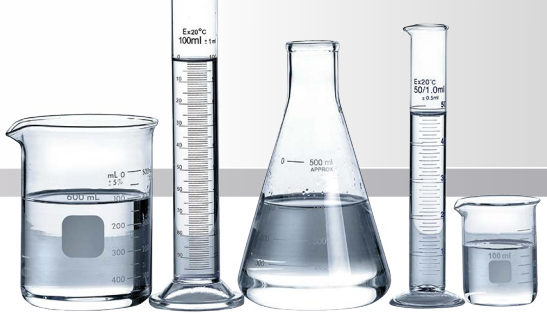
Advanced Detection Capabilities

RefractoMax 521 Refractive Index Detector

The Thermo Scientific RefractoMax 521 Refractive Index Detector from ERC Inc. This detector, in combination with the UltiMate 3000 system, is the right choice for the isocratic analysis of sugars, polymers, and fatty acids. It features fast baseline stabilization and excellent reproducibility, combined with high sensitivity. The RefractoMax 521 is fully controlled by Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System Software (CDS), and can also operate in stand-alone mode.

- The detector is highly sensitive and applicable universally. It provides very stable baselines with a drift of 0.2 µRIU/h and a noise specification of 2.5 nRIU or less
- The optical bench, thermostatically regulated from 30 °C to 55 °C, and the superior signal-to-noise ratio ensure highly precise measurement results
- The extended flow rate range from 1 mL/min up to 10 mL/min and the operating range of 1.00 to 1.75 RIU enable the use of this detector for a wide range of applications
- Applications include the analysis of all compounds with low UV-Vis activity, such as alcohols, mono- and polysaccharides, esters, fatty acids, or polymers
- An Auto Set-up function automates purging, equilibration, autozero, and the control baseline stability and noise
- Operation with Chromeleon CDS makes the detector easy to use and ensures maximum productivity in instrument control, data processing, and reporting of results

RefractoMax 521 Refractive Index Detector



Advanced Detection Capabilities

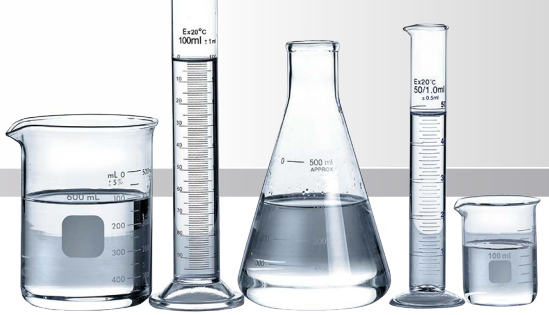
UltiMate 3000 Diode Array and Multiple-Wavelength Detectors

The Thermo Scientific Dionex UltiMate DAD 3000 detector is a high-resolution, 1024-element diode array detector (DAD) available in Rapid Separation (200 Hz) and Standard (100 Hz) versions. It operates with Chromeleon CDS software to provide a variety of spectra views, including 3-D plotting and automated chromatogram handling. The high resolution and low-noise performance of the DAD-3000 family makes it ideal for the most sensitive and accurate library searches and peak purity analyses.

The detector is also available as a multiple wavelength detector (MWD) in Standard (100 Hz) and Rapid Separation (200 Hz) versions.

- Data collection at up to 200 Hz using a maximum of eight single-wavelength data channels and one 3-D field (3-D only with DAD-3000 (RS)) for best support of ultrafast separations
- Standard versions operate at up to 100 Hz data collection rate for optimum support of 62 MPa (9000 psi) UltiMate 3000 Standard systems
- Accurate compound confirmation with a 1024-element, high resolution photodiode array
- Flexibility in both UV and Vis applications with 190–800 nm wavelength range
- Low-noise over the full spectral range using deuterium and tungsten lamps
- Fast and accurate wavelength verification using a built-in holmium oxide filter
- The detector can be upgraded with the UltiMate PCM 3000 for accurate monitoring pH gradients
- Excellent reliability and reproducibility with low baseline drift (typically < 500 µAU/h)
- Simplified routine maintenance with front access to pre-aligned cells and lamps
- ID chips on flow cells and lamps for identification and life-span monitoring
- Chromeleon CDS software for full control and flexible data handling
- Front-panel display for easy monitoring of detector status to maximize uptime
- Flow cells for semi-micro, semi-analytical, analytical, and semi-preparative applications
- Flow cells available in stainless steel and biocompatible versions

UltiMate 3000 DAD-3000 Diode Array Detector



Advanced Detection Capabilities

UltiMate 3000 Electrochemical Detector

Electrochemical detection delivers high sensitivity for neurotransmitter analysis, simplicity and robustness for pharmaceutical or clinical diagnostics, and the selectivity for the characterization of complex samples such as natural products, biological tissues and fluids. For today's researcher, there is a continuing need for detecting vanishingly small quantities of analyte and often in complex samples. Because electrochemical detection measures only compounds that can undergo oxidation or reduction it is both highly sensitive and very selective.

The Thermo Scientific Dionex UltiMate 3000 Electrochemical Detector, designed by the pioneers of coulometric electrochemical detection, delivers state-of-the-art sensor technologies complete with an entire range of high performance and ultra-high performance LC systems optimized for electrochemical detection. The UltiMate 3000 ECD-3000RS takes electrochemical detection to the next level with UHPLC compatibility, total system integration, and selection of detection mode, all with unprecedented operational simplicity.

Features include:

- Detection Modes – choose from DC and PAD for optimum analyte response
- Choice of sensors – both coulometric and amperometric sensors to meet the demands of any application
- UHPLC compatibility – ultralow peak dispersion and high data acquisition rates for conventional or fast, high resolution chromatography
- Modularity – easily expandable to multiple independent sensors for unrivaled flexibility
- Autoranging – simultaneously measure both low and high levels of analytes without losing data
- SmartChip™ technology – easy operation with automatic sensor recognition, event logging and electrode protection

UltiMate 3000 Electrochemical Detector

Thermo SCIENTIFIC

Learn more at www.thermoscientific.com/ECDetection

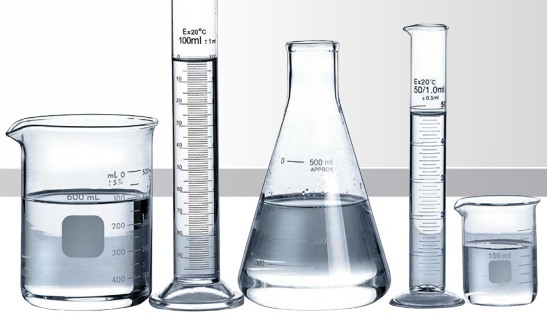


Table of Contents

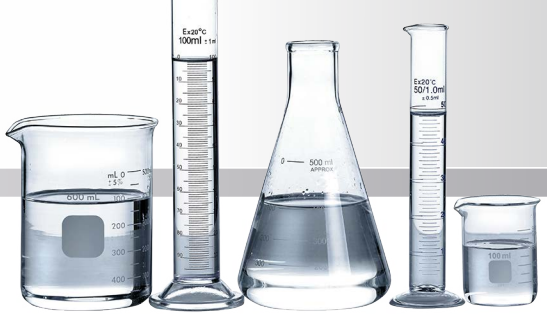
Advanced Detection Capabilities

UltiMate 3000 Fluorescence Detector

The Thermo Scientific Dionex UltiMate 3000 FLD-3000 is a high-sensitivity fluorescence detector series for UltiMate 3000 HPLC systems. It is available in Rapid Separation (RS) and Standard (SD) versions. The optics of the FLD-3000 series provide maximum stray-light suppression for best detection sensitivity. Operated with the Chromeleon CDS software, the detector provides automated qualification, various tools for method development, and instrument wellness monitoring for ease of use, maximum uptime, and the highest degree of regulatory compliance.

- Data collection at up to 200 Hz for optimal support of even the fastest UHPLC separations (FLD-3400RS)
- Standard detectors operate at up to 100 Hz data rate for optimum support of 62 MPa (9,000 psi) UltiMate 3000 standard systems
- Lowest limits of detection with a Raman signal-to-noise ratio (S/N): > 550 ASTM (> 2100 using dark signal as noise reference)
- Unsurpassed reproducibility with active flow cell temperature control for stable fluorophore activity independent of changes in ambient temperature
- Long-life xenon flash lamp for highest sensitivity and long-term operation without the need for frequent lamp changing
- Optional second photomultiplier (PMT) for unique Dual-PMT operation, offering an extended wavelength range up to 900 nm without sacrificing sensitivity in the standard wavelength range
- Two-dimensional (2D) or three dimensional (3D) excitation, emission, or synchro scans to provide the highest degree of flexibility for method development or routine sample characterization
- Innovative Variable Emission Filter for real-time compound-related sensitivity optimization (FLD-3400RS only)
- Large front-panel display for easy monitoring of the detector status
- Two flow-cell sizes for easy optimization to application requirements: the 8 µL flow cell is ideal for trace analysis, and the 2 µL flow cell offers best peak resolution with narrow-bore HPLC and UHPLC columns

Ultimate 3000 Fluorescence Detector



Advanced Detection Capabilities

UltiMate 3000 Variable Wavelength Detectors

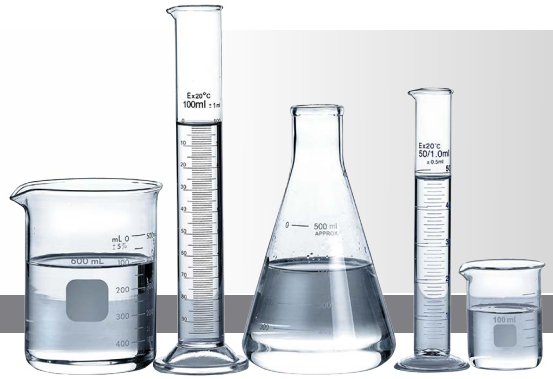
The Thermo Scientific Dionex UltiMate 3000 VWD-3000 is a variable wavelength detector (VWD) series for industry leading UV-Vis detection. The forward optics design and wide range of available flow cells ensure optimal performance over a flow rate range of five orders of magnitude. Automated qualification, performance optimization, and instrument wellness monitoring deliver maximum uptime, simplify work-flow, and give you full confidence in your analytical results. The detector is available in a standard 100 Hz (VWD-3100) and a 200 Hz Rapid Separation version (VWD-3400RS) for the most challenging UHPLC applications.

High-Performance UV-Vis Detection

- The VWD-3400RS variant provides data collection rates of up to 200 Hz for optimal support of today's and tomorrow's UHPLC separations
- The VWD-3100 standard detector operates at up to 100 Hz data rate for optimum support of 62 MPa (9000 psi) UltiMate 3000 Standard systems
- Superior detection of trace analytes with low noise (< –2.0 µAU) and drift (< 100 µAU/h)
- The detector's large linearity range of up to 2.5 AU is ideal for applications with widely varying analyte concentrations
- Up to four absorption channels (VWD-3400RS) and spectral scans support effective method development
- Active temperature control of optics and electronics for data acquisition independent of ambient conditions
- Front panel access for quick and easy lamps and flow cells changes
- Automated qualification monitoring for full regulatory compliance
- Large front panel display for monitoring the detector status even from a distance
- Maximize uptime using predictive performance–based on monitoring the life cycle of detector lamps
- The detector can be upgraded with the Thermo Scientific Dionex pH/Conductivity Monitor (PCM-3000) for accurate and precise pH- and conductivity monitoring
- Unique 45 nL ultra-low dispersion UV monitor for dispersion-free UV detection in LC/MS

UltiMate 3000 VWD-3400 Variable Wavelength Detector.

Table of Contents

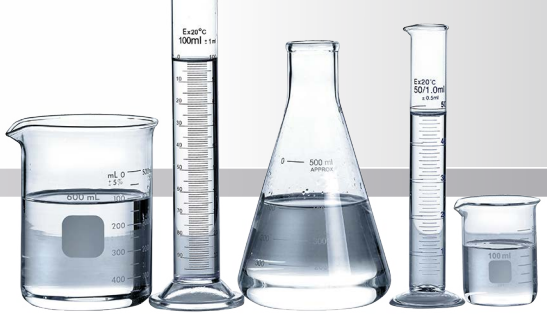


Analytical Technologies

Ion Chromatography

Thermo Scientific Dionex IC systems have led the analytical instrument industry for over 30 years with solutions that represent state-of-the art technological advancements and patented technologies.

Thermo SCIENTIFIC



IC and RFIC Systems

Table of Contents

Innovative Ion Chromatography Solutions

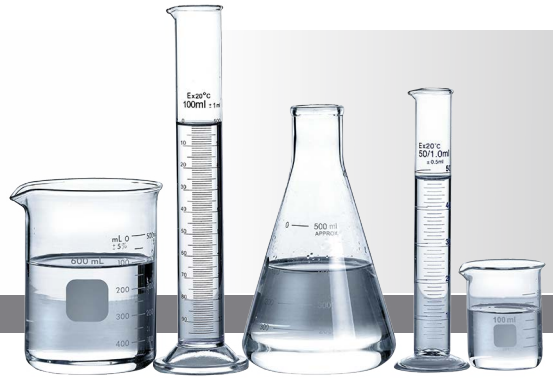
Our High-Pressure™ Ion Chromatography (HPIC™) systems include the Thermo Scientific Dionex ICS-5000+ HPIC system, which is optimized for flexibility, modularity, and ease-of-use, combining the highest chromatographic resolution with convenience. In addition, the Thermo Scientific Dionex ICS-4000 Capillary HPIC system is the world's first commercially available dedicated capillary high-pressure Reagent-Free™ (RFIC™) IC system. The Dionex ICS-4000 system is always ready for the next analysis, delivering high-pressure IC on demand.

Reagent-Free IC systems eliminate daily tasks of eluent and regenerant preparation in turn saving time, preventing errors, and increasing convenience. RFIC-EG systems use electrolytic technologies to generate eluent on demand from deionized water, and to suppress the eluent back to pure water to deliver unmatched sensitivity. RFIC-ER systems are designed to use carbonate, carbonate/ bicarbonate, or MSA eluents for isocratic separations.

At the heart of our ion chromatography portfolio is a unique set of column chemistries that provide high selectivities and efficiencies with excellent peak shape and resolution. Thermo Scientific™ Dionex™ IonPac™ chromatography columns address a variety of chromatographic separation modes including ion exchange, ion exclusion, reversed-phase ion pairing, and ion suppression. Our column chemistries are designed to solve specific applications, and we offer a variety of selectivities and capacities for simple and complex samples. Additionally, our Dionex IonPac column line is available in standard bore, microbore and capillary formats for the ultimate application flexibility.

Thermo Scientific Dionex IC instrument family

Table of Contents

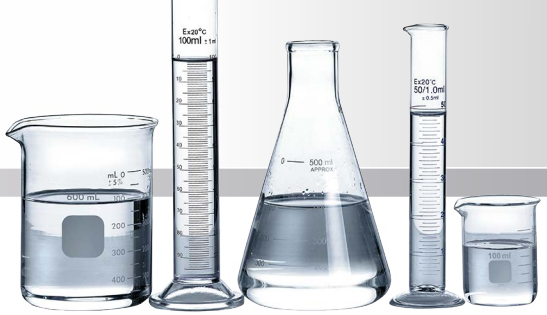


Analytical Technologies

Mass Spectrometry

We provide advanced integrated IC/MS and LC/MS solutions with superior ease-of-use and modest price and space requirements. UltiMate 3000 System Wellness technology and automatic MS calibration allow continuous operation with minimal maintenance. The Dionex ion chromatography family automatically removes mobile phase ions for effort-free transition to MS detection.

Thermo SCIENTIFIC



Mass Spectrometry Instruments

Single-Point Control and Automation

We provide advanced integrated IC/MS and LC/MS solutions with superior ease-of-use and modest price and space requirements. UltiMate 3000 System Wellness technology and automatic MS calibration allow continuous operation with minimal maintenance. The Dionex ion chromatography family automatically remove mobile phase ions for effort-free transition to MS detection.

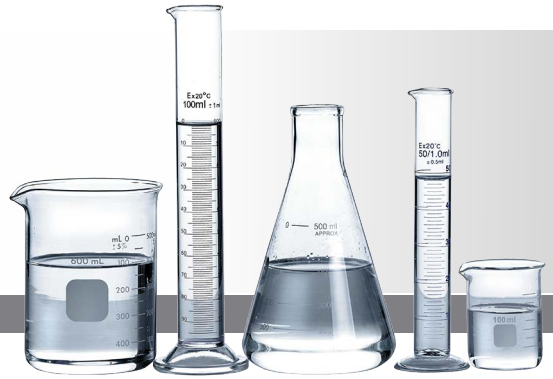
- Thermo Scientific™ MSQ Plus™ mass spectrometer, the smallest and most sensitive single quadrupole on the market for LC and IC
- Self-cleaning ion source for low maintenance operation
- Chromeleon CDS software for single-point method setup, instrument control, and data management compatible with existing IC and LC methods
- The complete system includes the MSQ Plus mass spectrometer, PC data system, electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) probe inlets, and vaccum system

Now, you no longer need two software packages to operate your LC/MS system. Chromeleon CDS software provides single-software method setup and instrument control; powerful UV, conductivity, and MS data analysis; and fully integrated reporting.

MSQ Plus Mass Spectrometer

Table of Contents

Table of Contents

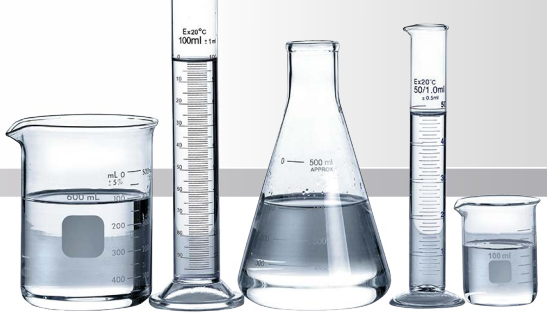


Analytical Technologies

Chromatography Data Systems

Tackle chromatography management challenges with the world's most complete chromatography software. Whether your needs are simple or complex or your scope is a single instrument, a global enterprise, or anything in between – the combination of Chromeleon CDS' scalable architecture and unparalleled ease-of use, makes your job easy and enjoyable with one Chromatography Data System for the entire lab.

Thermo SCIENTIFIC



Chromeleon CDS Software

Table of Contents

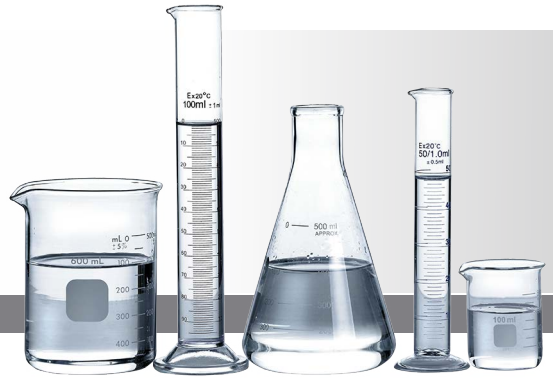
The Fastest Way from Samples to Results

The 7.2 release of Chromeleon Chromatography Data System software is the first CDS that combines separation (GC/IC/LC) and Mass Spectrometry (MS) in an enterprise (client/server) environment. By extending Chromeleon 7.2 CDS beyond chromatography into MS, lab technicians can now streamline their chromatography and MS quantitation workflows with a single software package. MS support in Chromeleon 7.2 CDS is focused on routine and quantitative workflows, which provides access to rich quantitative data processing and automation capabilities — ultimately boosting your overall lab productivity and increasing the quality of your analytical results.

- Enjoy a modern, intuitive user interface designed around the principle of operational simplicity
- Streamline laboratory processes and eliminate errors with eWorkflows™, which enable anyone to perform a complete analysis perfectly with just a few clicks
- Access your instruments, data, and eWorkflows instantly in the Chromeleon Console
- Locate and collate results quickly and easily using powerful built-in database query features
- Interpret multiple chromatograms at a glance using MiniPlots
- Find everything you need to view, analyze, and report data in the Chromatography Studio
- Accelerate analyses and learn more from your data through dynamic, interactive displays
- Deliver customized reports using the built-in Excel® compatible speadsheet

Thermo SCIENTIFIC

Table of Contents

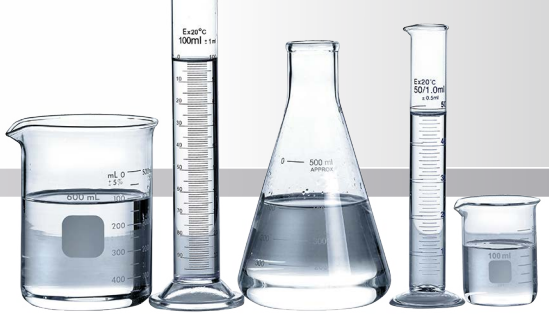


Analytical Technologies

Process Analytical Systems

Thermo Scientific Dionex process analytical systems provide timely results by moving chromatography-based measurements on-line.

Thermo SCIENTIFIC



Process Analytical Systems and Software

Improved Process Monitoring with On-line Chromatography IC and LC Systems

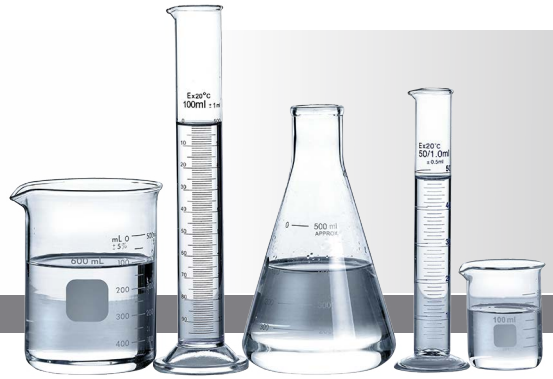
Information from the Thermo Scientific Dionex Integral process analyzer can help reduce process variability, improve efficiency, and reduce downtime. These systems provide comprehensive, precise, accurate information faster than is possible with laboratory-based results. From the lab to the factory floor, your plant's performance will benefit from the information provided by on-line LC.

- Characterize your samples completely with multicomponent analysis
- Reduce sample collection time and resources with automated multipoint sampling
- Improve your process control with more timely results
- See more analytes with unique detection capabilities
- The Thermo Scientific Integral Migration Path approach lets you choose the systems that best meets your needs

Integral process analyzer

Table of Contents

Table of Contents

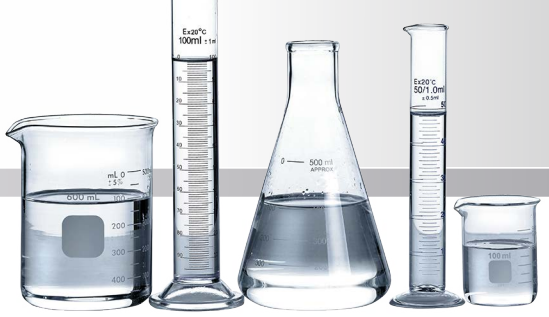


Analytical Technologies

Automated Sample Preparation

Solvent extractions that normally require labor-intensive steps are automated or performed in minutes, with reduced solvent consumption and reduced sample handling using the Thermo Scientific™ Dionex™ ASE™ Accelerated Solvent Extractor system or Thermo Scientific™ Dionex™ AutoTrace™ 280 Solid-Phase Extraction instrument.

Thermo SCIENTIFIC



Accelerated Solvent Extractor System

Table of Contents

Complete Extractions in Less Time Using Less Solvent

Thermo Scientific Dionex ASE systems extract of solid and semisolid samples using common solvents at elevated temperature and pressure. The Dionex ASE 150 and 350 systems feature pH-hardened pathways with Dionium™ components to support extraction of acidic or alkaline matrices, and combine pretreatment, solvent extraction, and cleanup into one step. Dionium is zirconium that has undergone a proprietary hardening process that makes it inert to chemical attack by acids and bases at elevated temperatures.

Dionex ASE systems are dramatically faster than Soxhlet, sonication, and other extraction methods, and require significantly less solvent and labor. Accelerated solvent extraction methods are accepted and established in the environmental, pharmaceutical, foods, polymers and consumer product industries. Accelerated solvent extraction methods are accepted and used by government agencies worldwide.

Dionex ASE 150/350 and Dionex AutoTrace 280 SPE instruments

Table of Contents

Profiling Beverages

English "bitter" ale

Beer

The first step in the beer making process involves soaking barley, and sometimes other grains, in warm water. Enzymes present in the barley break down starch from the grains, producing mostly glucose, maltose, and oligo- and polysaccharides. This process is called mashing, and the resulting solution is called sweet wort. The sweet wort is then treated with hops, thereby producing hopped wort. Yeast is added and the smaller saccharides are fermented to produce alcohol.

Thermo SCIENTIFIC

Beer: Carbohydrates

Because of the different concentrations, chemical behavior, and molecular mass ranges otf the various components in beer, their isolation and determination can be difficult. Ion chromatography, using polymer-based resins, provides a means to monitor many of these important compounds during the brewing process and in the final product.

This application describes the use of ion-exchange or ion-exclusion chromatography for the determination of five classes of compounds of interest to the brewing industry, including: carbohydrates, alcohols, organic acids, inorganic anions, and inorganic cations. One of two forms of electrochemical detection is used, pulsed amperometry or conductivity detection.

Column:	Dionex CarboPac PA1			
Flow:	1.0 mL/min			
Injection Volume:	10 µL			
Mobile Phase:	A. Deionized water			
	B. 500 mM Sodium hydroxide			
Gradient:	Time	%A	%B	Comments
	Initial	99	1	Reequilibrate
	5.00	99	1	Inject
	6.00	99	1	Back to Load
	20.00	91	9	
	45.00	0	100	
	50.00	0	100	
Detection:	Pulsed amperometry, gold electrode			

Peaks:
1. Glucose
2. Fructose
3. Isomaltose
4. Sucrose
5. Maltose
6. Maltoriose

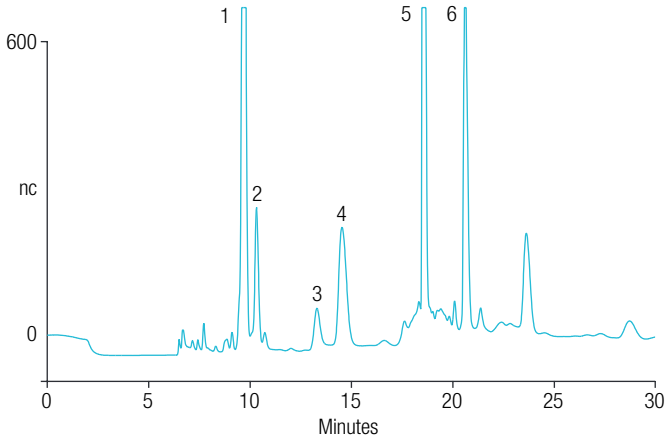


Figure 6-1. Separation of fermentable sugars in wort by ion exchange chromatography with pulsed amperometric detection.

Column:	Dionex CarboPac PA1			
Flow:	1.0 mL/min			
Injection Volume:	10 µL			
Mobile Phase:	A. Deionized water			
	B. 500 mM Sodium hydroxide			
Gradient:	Time	%A	%B	Comments
	Initial	99	1	Reequilibrate
	5.00	99	1	Inject
	6.00	99	1	Back to Load
	20.00	91	9	
	45.00	0	100	
	50.00	0	100	
Detection:	Pulsed amperometry, gold electrode			

Peaks:
1. Glucose
2. Fructose
3. Isomaltose
4. Sucrose
5. Maltose
6. Maltoriose

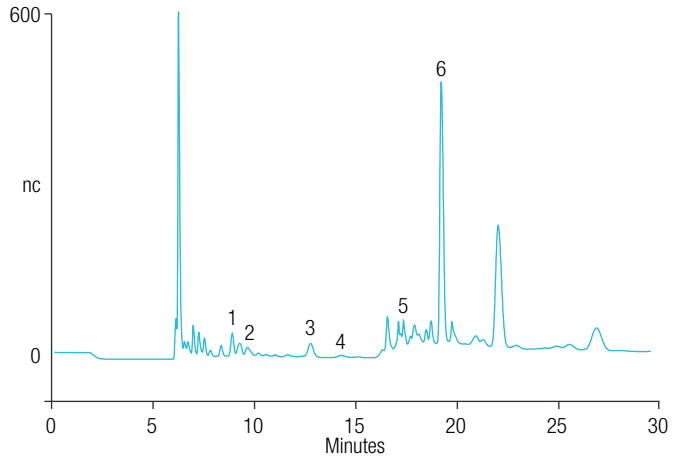


Figure 6-2. Separation of mono-, di-, and trisaccharides in an American beer by ion-exchange chromatography with pulsed amperometric detection.

Thermo SCIENTIFIC

Beer: Carbohydrates

Determining the levels of fermentable and non-fermentable sugars at every stage of beer production is important because fermentable sugars determine the final alcohol content, and nonfermentable sugars contribute to the flavor and "body" of the final product.

Table of Contents

Column:	Dionex CarboPac PA-100				
Flow:	1.0 mL/min				
Injection Volume:	10 µL				
Mobile Phase:	A. Deionized water				
	B. 500 mM Sodium hydroxide				
	C. 1 M Sodium acetate				
Gradient:	Time	%A	%B	%C	Comments
	Initial	57	33	10	Reequilibrate
	1.50	57	33	10	Inject
	6.50	57	33	10	Gradient Start
	31.50	42	33	25	Gradient End
Detection:	Pulsed amperometry, gold electrode				

Peaks: 1. Ethanol
2. Glucose
3. Maltose
4. Maltoriose
5–11. Maltose oligomers

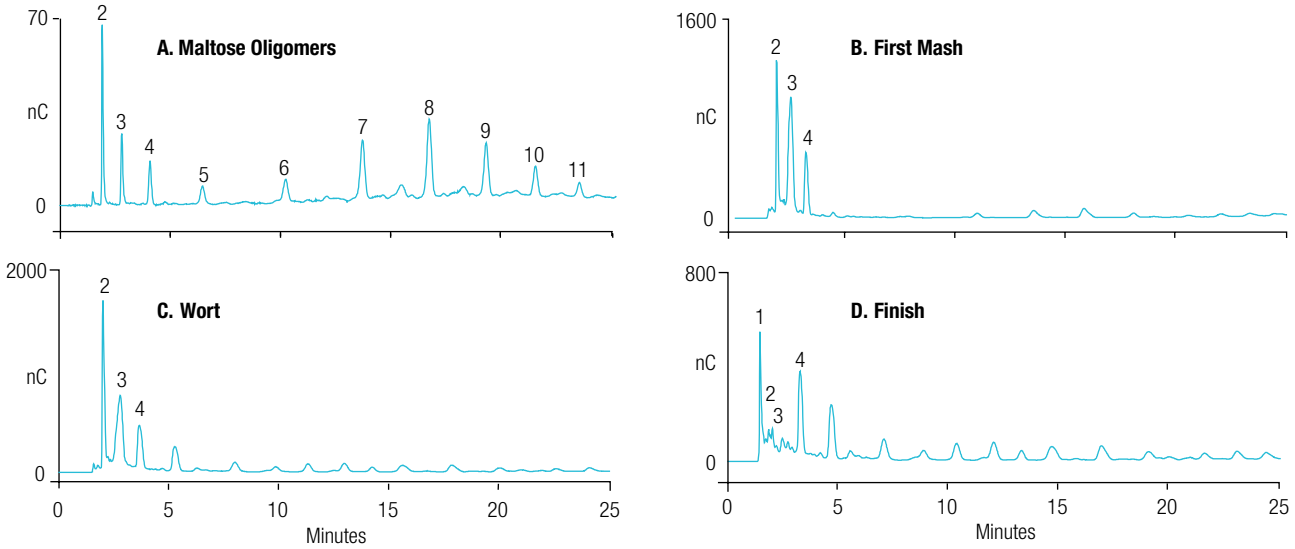


Figure 6-3. Sugar and oligosaccharide profiles during beer production. In panel A, maltose oligomers are baseline-separated. Chromatograms B, C, and D illustrate sugar and oligosaccharide profiles at different stages of the brewing process.

Thermo SCIENTIFIC

Beer: Chalcinoids and Bitter Acids

Table of Contents

Beer is the most widely consumed alcoholic beverage in the world and the third most popular drink after water and tea. It is typically brewed from four basic ingredients: water, a starch source such as malted barley, brewer's yeast, and a flavoring agent such as hops. Many varieties of beer result from differences in these ingredients, the additives used, and the brewing process followed.

Hops are the female flower clusters of a hop species, *Humulus lupulus*. They are used as a flavoring and stability agent in beer, for various purposes in other beverages, and as an herbal medicine. Hops contain a number of important phytochemicals including xanthohumol (a prenylated chalconoid) and alpha- and beta-acids. As part of the beer brewing process, hops or hop extracts are added during the boiling of the wort. The alpha-acids (humulone, cohumulone, and adhumulone) are slowly isomerized into the more soluble iso-acids, the main bittering substances in beer. Beta-acids (lupulone, colupulone, and adlupulone) do not isomerize during boiling and do not impart bitterness initially. However, during fermentation and storage, beta-acids slowly create bitterness through oxidation affecting the long-term character of aged beers. Furthermore, some secondary metabolites contribute to the degradation of beer during storage with the formation of haze (e.g., catechins and their polymers, the proanthocyanidins).

Pump:	LPG-3400BM with SR-3000 solvent rack
Autosampler:	WPS-3000TBSL
UV Detector:	DAD-3000RS diode-array detector
	Channel 1: 218 nm Channel 2: 240 nm
	Channel 3: 254 nm Channel 4: 275 nm
EC Detector:	CoulArray detector with thermal organizer
EC Parameters:	Model 5011A dual channel coulometric electrochemical cell
	E1: +550 mV
	E2: +850 mV
Column:	Acclaim 120, C18 (3.0 × 150 mm, 3 µm particle size)
Flow:	0.65 mL/min
Injection Volume:	20 µL
Mobile Phase:	A. 25 mM sodium perchlorate, 50% acetonitrile, 2.5 mM perchloric acid
	B. 25 mM sodium perchlorate, 90% acetonitrile, 2.5 mM perchloric acid
	C. 90% methanol
Gradient:	0-3 min: 0%B/3%C, 30 min: 40%B/3%C, 40 min: 97%B/3%C, 45 min: 97%B/3%C

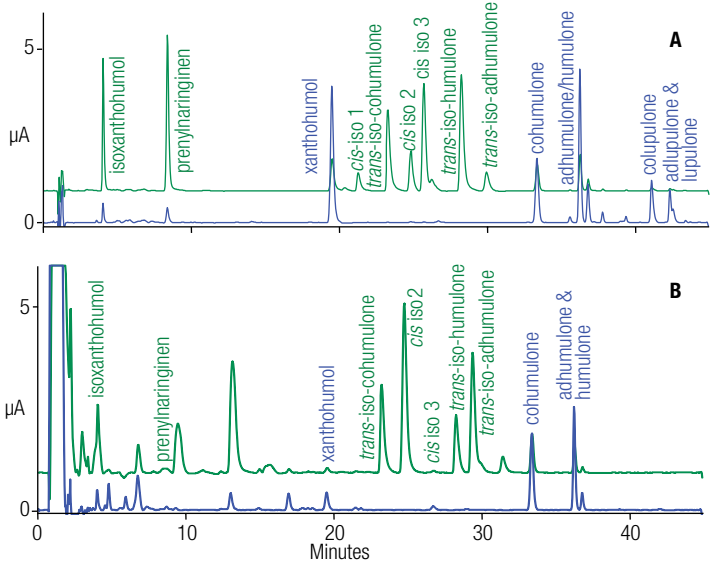


Figure 6-4. Chromatograms of (A) bitter acids standard mixture; (B) Ultra IPA beer sample. Blue trace at 550 mV; green trace at 850 mV. The *cis*-isomers were *cis*-rho-isocohumulone, *cis*-rho-isohumulone, and *cis*-rho-isoadhumulone.

Thermo SCIENTIFIC

Beer: Chalcinoids and Bitter Acids

Application Note 1020 describes how gradient HPLC with selective and sensitive Spectro-Electro Array detection, can be used to simultaneously measure many chalcinoids and bitter acids in beer samples, without the need for solid phase extraction. This approach can also be used to study beer stability.

Table 6-1. Hops bitter acids data presented in mg/L.

Compound	Beer 1 Ultra IPA	Beer 2 Ultra IPA	Beer 3 Regular	Beer 4 Light Beer
Isoxanthohumol	2.10	1.3	0.38	0.28
Xanthohumol	0.52	0.48	ND	ND
cis-iso-acid 1	0.90	0.4	ND	ND
trans-iso-cohumulone	10.6	7.0	ND	ND
cis-iso-acid 2	19.1	12.2	3.8	1.6
trans-iso-humulone	8.4	7.6	0.20	ND
trans-iso-adhumulone	12.8	11.0	3.2	2.6
Cohumulone	6.8	6.4	0.03	0.02
Adhumulone/Humulone	9.2	9.0	ND	ND

Did You Know?

According to a diary entry from a passenger on the Mayflower, the pilgrims made their landing at Plymouth Rock, rather than continue to their destination in Virginia, due to lack of beer.

Table of Contents

Thermo SCIENTIFIC

Download Application Note 1020: Chalconoids and Bitter Acids in Beer by HPLC with UV and Electrochemical Detection

Beer: Iso-alpha Acid Analysis

Isohumulones (iso-α-acids) are derived by humulones (α-acids), essential constituents of hop resins. The poorly water-soluble α-acids are isomerized to the better water-soluble iso-α-acids during wort-boiling. Iso-α-acids form approximately eighty percent of the typical bitterness of beer. Their antimicrobial effect leads to a sterile beverage, their tensioactive character stabilizes the foam, and they have a major influence on the general flavor, smell, and smoothness of beer.

The three major iso-α-acid variants which are basically present in beer only differ in their acyl side chain and comprise iso-nhumulone, iso-cohumulone, and iso-adhumulone. Due to the stereochemistry of iso-α-acids, all of them occur as cis- and trans-isomers. Each iso-α-acid variant provides different contributions to beer taste and foam stability. Recent investigations have shown that these differences are even true between both cis- and trans-isomers of the same iso-α-acid. Furthermore, the lifetimes of cis- and trans-isomers significantly differ from each other. Degradation products of iso-α-acids influence the important beer attributes mentioned above and the avoidance of less stable iso-α-acid variants is beneficial.

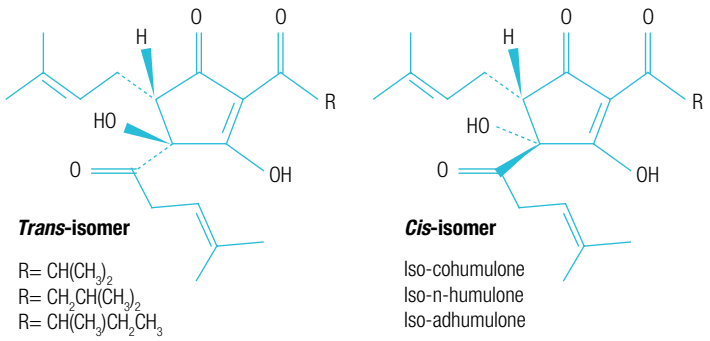


Figure 6-5. Chemical structures of *cis*- and *trans*-iso-α-acids.

Application Brief 153 describes a rapid HPLC-UV method with on-line sample preparation for the routine analysis of bitter acids in beer samples.

System:	UltiMate 3000 System with On-Line SPE RS Configuration
Temperature:	35 °C
Injection Volume:	15 µL beer (orange trace) or 5 µL isohumulone standard (purple trace)
Mobile Phase:	A. Water with 1% formic acid and 100 mg/L ethylenediaminetetraacetic acid disodium salt dihydrate B. Acetonitrile
Pressure:	720 bar (max.)

Analytical Flow Path Parameters

Column:	Hypersil GOLD column, 1.9 µm, 100 × 2.1 mm
Flow:	650 µL/min
Isocratic:	50% B
Detection:	UltiMate VWD-3400RS Variable Wavelength Detector, 2.5 µL flow cell, 270 nm

Automated On-Line SPE Parameters

Column:	Hypersil GOLD C8 column, 5 µm, 20 × 2.1 mm
Gradient:	0–2 min 25% B at 2000 µL/min, 2–4 min 100% B at 2000 µL/min, 4–7 min 25% B at 200 µL/min, 7–9 min 25% B at 2000 µL/min
Valve Position:	0 min 6_1, 1.5 min 1_2, 2 min 6_1

Analytes:
1. *Trans*-iso-cohumulone
2. *Cis*-iso-cohumulone
3. *Trans*-iso-n-humulone
4. *Cis*-iso-n-humulone
5. *Trans*-iso-adhumulone
6. *Cis*-iso-adhumulone

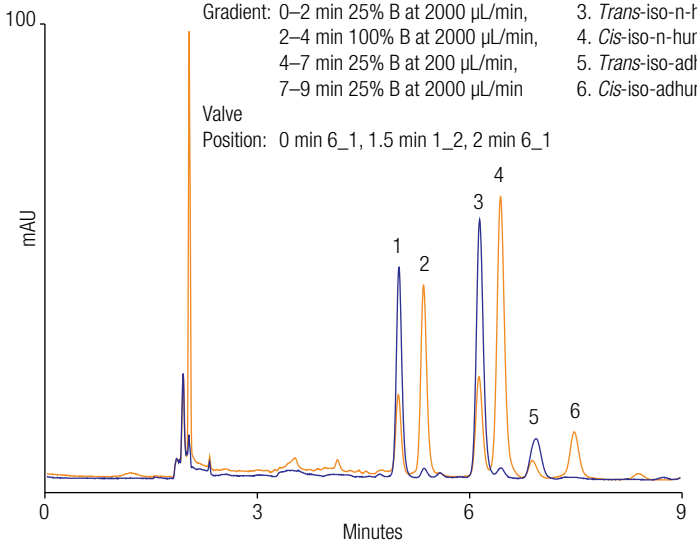


Figure 6-6. Chromatogram of isohumulones in beer and isohumulones standard (overlay).

Download Application Brief 153: Save the Flavor — Robust Iso-α-Acids Assaying in Beer within Ten Minutes

Table of Contents

Beer: Glutamate

Glutamate is naturally present in low concentrations in beer and is also a legal flavor additive in some jurisdictions. This assay is quick, selective, and automates all the sample preparation. The Acclaim PA column provides high resolution, even in this complex sample.

Column:	Acclaim PA, C16 5 µm, 4.6 × 50 mm
Flow:	1.5 mL/min
Temperature:	30 °C
Injection Volume:	20 µL
Mobile Phases:	(A) Methanol
	(B) 20 mM phosphate, pH 7.0
Gradient Times:	0.0 2.0 3.0 5.0 5.1 6.5
	%A: 10 30 75 75 10 10
	%B: 90 70 25 25 90 90
Detector:	UVD 340U; UV at 330nm and spectra 200–400 nm
Samples:	(A) Beer
	(B) Beer + 250 µg/mL glutamic acid
Derivatizing Conditions:	(Reagent A) 2 mg/mL o-phthalaldehyde n 0.5M borate buffer, pH 10.4
	(Reagent B) 6 mg/mL $(CH_3)_2NCH_2CH_2SH$ HCl in water
Program:	75 µL reagent A + 75 µL reagent B + 15 µL sample, mixed in round-bottom glass vial
Reaction Time:	5 min at room temperature

Did You Know?

- A collector of beer bottles is called a labeorphilist
- A beer lover or enthusiast is called a cerevisaphile
- Cenosillicaphobia is the fear of an empty glass

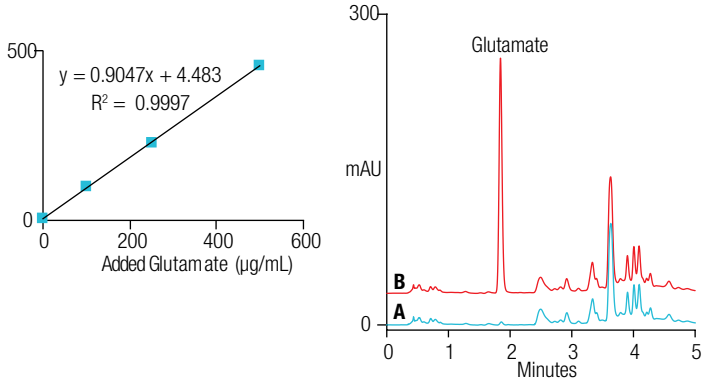


Figure 6-7. Glutamate in beer by automated precolumn OPA derivatization.

Thermo SCIENTIFIC

Beer: Organic Acids

Beer production has been of interest since the beginnings of civilization with brewing processes advancing along with society. Beer is a complex sample matrix that contains numerous components including proteins, carbon dioxide, carbohydrates, inorganic anions and cations, aldehydes, organic acids, and ethanol. These can be passively introduced from the minerals in the water, extracted from the brewing ingredients, generated in the fermentation process, or added to achieve a desired characteristic flavor.

Organic acids are end products of yeast fermentation critical to the flavor of beer, but are also products of bacterial fermentation that introduce a sour flavor, either purposely or unintentionally due to spoilage.

Technical Note 126 describes the advantages of the 4 µm particle-size Dionex IonPac AS11-HC-4µm column combined with the Dionex ICS-5000$^+$ HPIC system for optimal separation of organic acids and inorganic anions in beer samples using electrolytically generated hydroxide eluent with and without an organic modifier.

Trivia Question

Q: Do you know where the word “bridal” originates from?

A: The word “bridal” comes from 19th century Englishmen, who took out their friends for a final “Bride Ale” the day before their wedding.

Column:	Dionex IonPac AS11-HC-4µm set, 2 × 250 mm
Flow:	0.38 mL/min
Temperature:	30 °C
Injection Volume:	2.5 µL
Eluent Source:	Dionex EGC 500 KOH cartridge; Channel A, Water Channel B, Methanol
Gradient :	1 mM KOH, 2% methanol (8 min), 2–10% methanol (8–8.1 min) 1–15 mM KOH, 10% methanol (8–18 min), 15–30 mM KOH,10% methanol (18–28 min), 30–60 mM KOH, 10% methanol (28–38 min)
Detection:	Suppressed conductivity, Dionex ASRS 300 suppressor, 4 mm, AutoSuppression, recycle mode
Sample Prep.:	5-fold dilution
Samples:	A: Lager beer 2; Sample, B: Sample A plus 10 ppm butyrate; C: Standard

Peaks (Standard):	mg/L				
1. Quinate	5	4. Acetate	5	13. Malate	10
2. Fluoride	3	5. Propionate	5	14. Tartrate	10
3. Lactate	5	6. Formate	5	15. Sulfate	10
		7. Butyrate	5	16. Fumarate	10
		8. Pyruvate	10	17. Oxalate	10
		9. Chloride	5	18. Phosphate	15
		10. Bromide	5	19. Citrate	15
		11. Nitrate	5	20. Isocitrate	15
		12. Succinate	10	21. *cis*-Aconitate	–
				22. *trans*-Aconitate	15

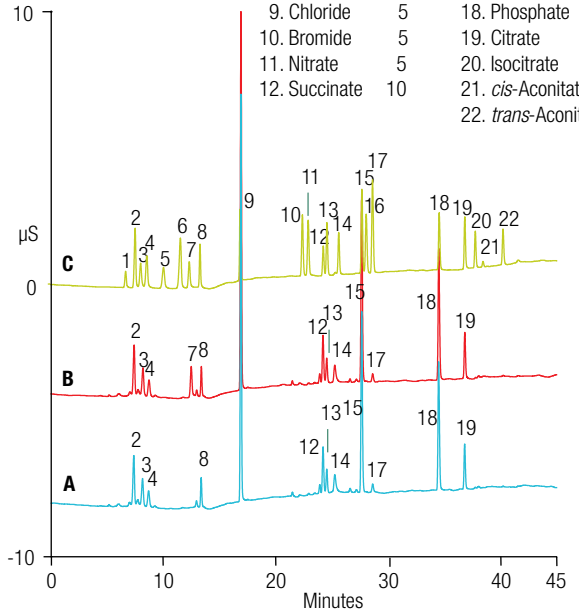


Figure 6-8. Analysis of Lager (A and B) and Light Larger (C) samples on a 4 mm i.d. column.

Download Technical Note 126: Determination of Organic Acids in Beer Samples Using an HPIC System

Table of Contents

Profiling Beverages

Carbonated Beverages

The determination of inorganic anions and cations and organic acids in non-alcoholic carbonated beverages is of importance from both health-related and manufacturing perspectives.

Thermo SCIENTIFIC

Carbonated Beverages: Acidulants

Acidulants reduce the soft drink's pH and thereby assist in beverage preservation for long-term storage. Acidulants can also be used as chelating agents, buffers, coagulators, and flavoring agents. In the latter role, the acidulant imparts a tart taste. The most common acidulants used in soft drinks are phosphoric and citric acids. Phosphoric acid is more effective in lowering the pH than organic acids, while citric acid produces a stronger tartness. Phosphoric acid is commonly found in colas whereas citric acid is typically added to fruit flavored beverages. However, these acids may be used alone or blended together to produce a more distinctive taste.

The National Soft Drink Association estimates that a modern bottling facility can produce as many as 2,000 cans of soft drinks per minute on each line of operation. This results in the production of nearly three million cans of soft drinks per day. To maintain product consistency and quality, it is critical that an accurate amount of acidulant is used for each production line and bottling facility. This requires a rapid, accurate, and rugged analytical method to confirm that an appropriate amount of phosphoric and/or citric acid has been added to the soft drink formulation.

Application Note 169 describes a reliable and rapid ion chromatography suppressed conductivity method for the analysis of phosphate and citrate in carbonated soft drinks.

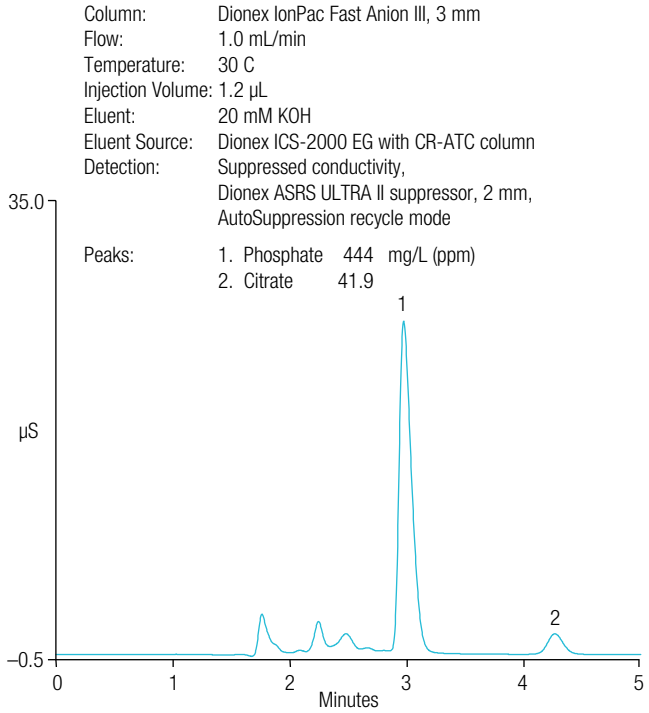


Figure 6-9. Determination of phosphate and citrate in a low-carbohydrate cola on the Dionex IonPac Fast Anion III column.

Download Application Note 169: Rapid Determination of Phosphate and Citrate in Carbonated Soft Drinks Using an RFIC System

Carbonated Beverages: Acidulants

Table of Contents

Column:	Dionex IonPac Fast Anion III, 3 mm
Flow:	1 mL/mn
Temperature:	30 C
Injection Volume:	1.2 µL
Eluent:	20 mM KOH
Eluent Source:	Dionex ICS-2000 EG with CR-ATC column
Detection:	Dionex ASRS ULTRA II suppressor, 2 mm, AutoSuppression recycle mode
Peaks:	1. Phosphate 540 mg/L (ppm)

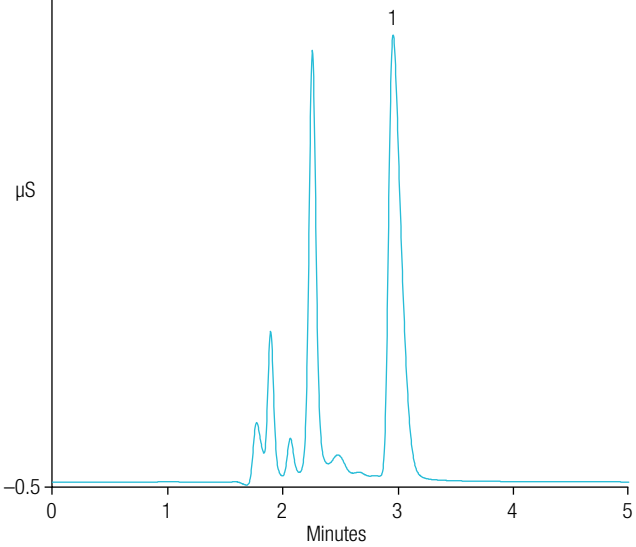


Figure 6-10. Determination of phosphate in a regular cola on the Dionex IonPac Fast Anion III column.

Thermo SCIENTIFIC

Carbonated Beverages: Inorganic Anions

Organic acids such as citrate and malate, and inorganic anions such as phosphate are monitored due to their function as acidifiers or flavor enhancers. Chloride is monitored due to restrictions imposed by different countries and many Group I and II metals are monitored for purposes of mass balance. Thus, the content of these compounds needs to be monitored by the manufacturer to maintain product quality and to investigate possible patent infringements in competitive products.

Column:	Dionex IonPac AS11 Analytical (4 mm) Dionex IonPac AG11 Guard (4 mm) ATC-1 Anion trap
Flow:	2 mL/min
Injection Volume:	25 µL
Detection:	Suppressed conductivity, Dionex ASRS 300 Suppressor, external water mode

Eluent: A. Deionized water
B. 1 mM Sodium hydroxide
C. 100 mM Sodium hydroxide
D. Methanol

Gradient:

Time	E1	E2	E3	E4
Initial	80	20	—	—
0.00	80	20	—	—
5.00	66	20	—	14
18.00	42	—	38	20

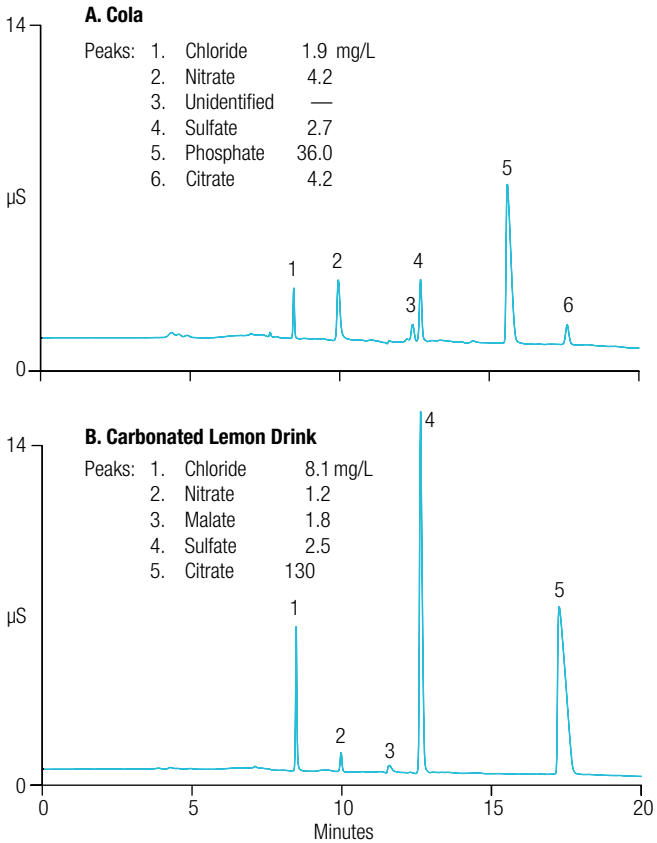


Figure 6-11. Separation of inorganic anions and organic acids in A) a cola and B) a carbonated lemon drink.

Did You Know?

Coca-Cola® was originally created by a chemist searching for a headache and hangover remedy. John Pemberton added kola nut extract to coca extract to produce Coca-Cola.

Thermo SCIENTIFIC

Carbonated Beverages: Inorganic Anions

Ion chromatography is a well established technique for the determination of ions in solution. Application Note 25 describes the use of ion exchange or ion exclusion chromatography (ICE) with suppressed conductivity detection for the determination of inorganic anions, cations, and organic acids in several popular carbonated beverages.

Did You Know?

The term seltzer used to refer to effervescent mineral water obtained from natural springs in Germany. Now, seltzer is used to describe well-filtered water with added artificial carbonation.

Column:	Dionex IonPac AS11 Analytical (4 mm)	Eluent:	A. Deionized water					
	Dionex IonPac AG11 Guard (4 mm)		B. 1 mM Sodium hydroxide					
	ATC-1 Anion trap		C. 100 mM Sodium hydroxide					
Flow:	2 mL/min		D. Methanol					
Injection Volume:	25 µL	Gradient:	Time	E1	E2	E3	E4	
Detection:	Suppressed conductivity,		Initial	80	20	—	—	
	Dionex ASRS suppressor,		0.00	80	20	—	—	
	external water mode		5.00	66	20	—	14	
			18.00	42	—	38	20	

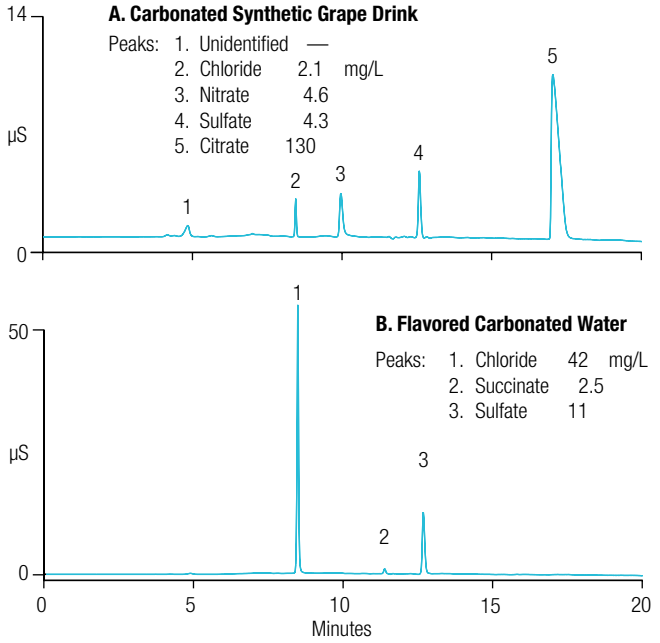


Figure 6-12. Separation of inorganic anions and organic acids in A) a carbonated synthetic grape drink and B) a synthetic carbonated water.

Download Application Note 25: Determination of Inorganic Ions and Organic Acids in Non-Alcoholic Carbonated Beverages

Carbonated Beverages: Inorganic Cations

Column:	Dionex IonPac CS12 Analytical (4 mm) Dionex IonPac CG12 Guard (4 mm) CTC-1 Cation trap
Flow:	1.0 mL/min
Injection Volume:	25 µL
Eluent:	1. Deionized water 2. 100 mM Methanesulfonic acid
Gradient:	Time E1 E2 Initial 84 16 5.00 84 16 5.01 60 40 10.00 60 40
Detection:	Suppressed conductivity, Dionex CSRS suppressor, recycle mode

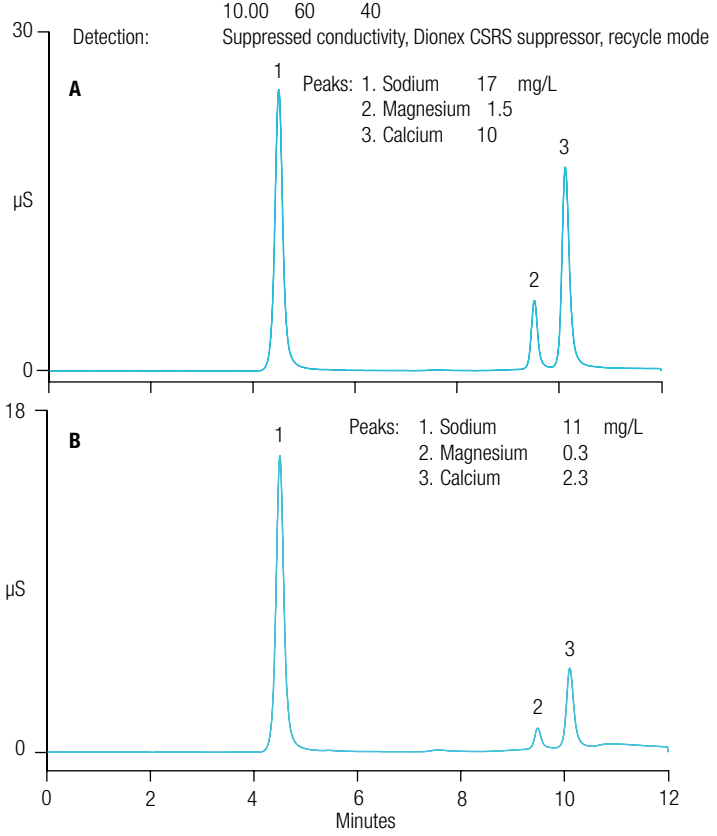


Figure 6-13. Separation of inorganic cations in A) a carbonated lemon drink and B) a carbonated synthetic grape drink.

For chromatographic conditions see Figure 6-14A

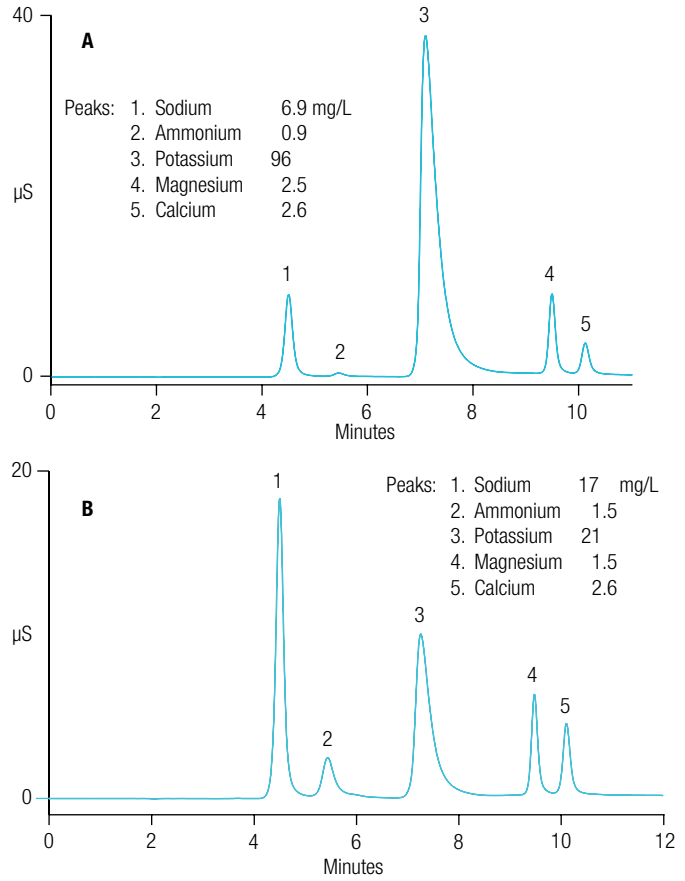


Figure 6-14. Separation of inorganic cations in A) a carbonated apple drink and B), a carbonated grape juice.

Carbonated Beverages: Organic Acids

Column: Dionex IonPac ICE-AS6 Analytical
Flow: 1.0 mL/min
Injection Volume: 25 µL
Eluent: 0.8 mM Heptafluorobutyric acid
Detection: Suppressed conductivity, Thermo Scientific™ Dionex™ AMMS-ICE™ 300 Anion-ICE MicroMembrane Suppressor
Regenerant: 5 mN Tetrabutylammonium hydroxide at 5 mL/min

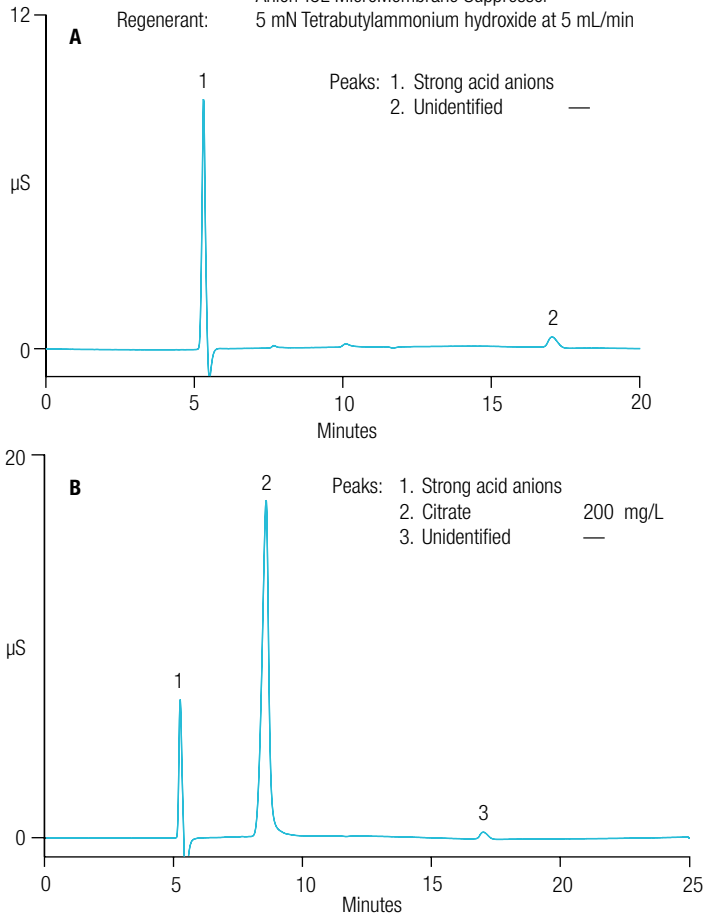


Figure 6-15. Separation of inorganic anions and organic acids in A) a flavored carbonated water and B) a carbonated lemon drink.

For chromatographic conditions see Figure 6-18A

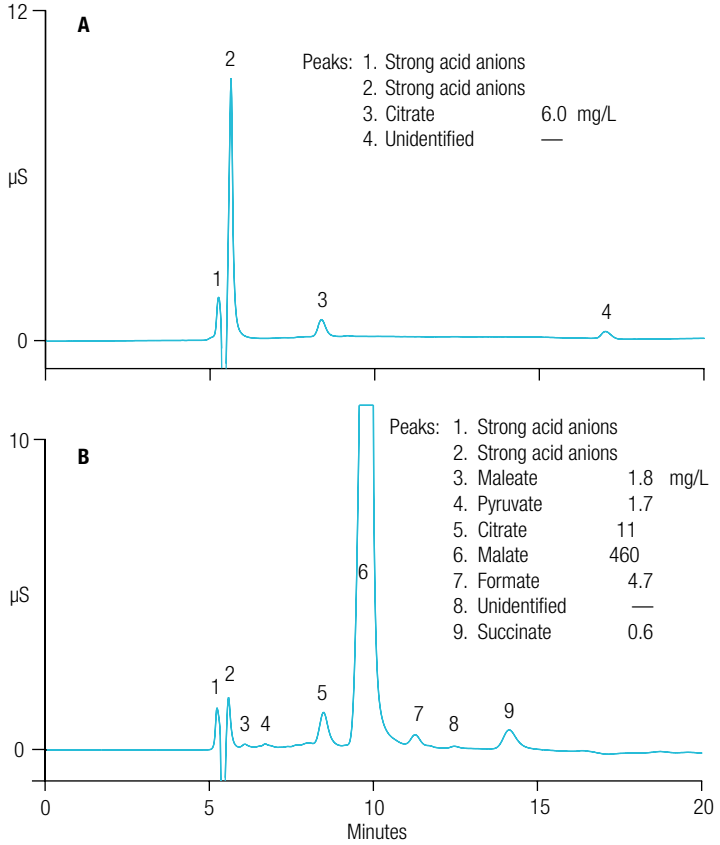


Figure 6-16. Separation of inorganic anions and organic acids in A) a cola and B) carbonated apple drink.

Thermo SCIENTIFIC

Table of Contents

Profiling Beverages

Coffee

Brewed coffee, one of the most popular beverages worldwide, is prepared from fermented and roasted coffee plant seeds (beans), typically *Coffea arabica* (Arabica). *Coffea canefora, variant robusta* (Robusta), provides a less desirable flavor, is less costly, and therefore is often blended or adulterated in Arabica to create less expensive coffees or to increase profits.

Thermo SCIENTIFIC

Coffee: Carbohydrates

Coffee carbohydrates constitute the major part (at least 50% of the dry weight) of raw coffee beans. The carbohydrates in coffee contribute to the flavor of the beverage as they undergo complex changes (react with amino acids, i.e., the Maillard reaction) during the roasting process. They act as aroma binders, foam stabilizers, and also impart viscosity to the coffee beverage. Carbohydrates are also good tracers for assessing the authenticity of soluble (instant) coffee.

Currently, the Association of Analytical Chemists (AOAC) official method 995.13 – which is based on high-performance anion-exchange (HPAE) chromatography with pulsed amperometric detection (PAD) – is used for determining the free and total carbohydrates in instant coffee. This method is also used by the British Standards Institution for testing coffee and coffee products. Application Note 280 compares a fast IC-PAD method to the official AOAC method 995.13.

Did You Know?

Coffee is the second largest traded commodity in the world, with oil being the largest. Specialty coffee revenue in 2006 topped $12.2 billion in sales.

Column:	Dionex CarboPac PA1 Analytical (4 × 250 mm), Dionex CarboPac PA1 Guard (4 × 50)	Peaks: 1. Mannitol 2. Fucose 3. Arabinose 4. Rhamnose 5. Galactose 6. Glucose 7. Xylose 8. Sucrose 9. Mannose 10. Fructose 11. Ribose
Flow:	1.0 mL/min	
Temperature:	15 °C	
Injection Volume:	10 µL	
Eluent:	DI water from 0–50 min 300 mM NaOH from 50–65 min DI water from 65-80 min (re-equilibration)	
Detection:	PAD (Au)	
Postcolumn Reagent:	300 mM Hydroxide	
PCR Flow Rate:	0.6 mL/min	
Traces:	A) Standards B) Free carbohydrates in green coffee C) Free carbohydrates in instant coffee D) Total carbohydrates in instant coffee	

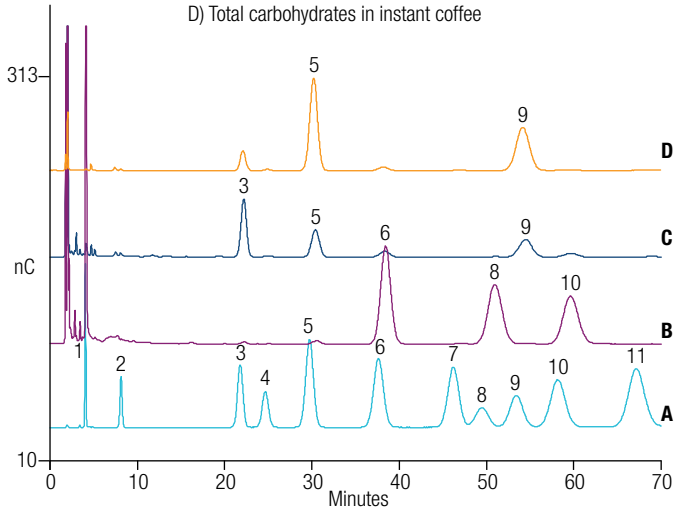


Figure 6-17. Chromatograms of mixed coffee carbohydrate standards (A), free carbohydrate in extract of green coffee beans (B), free carbohydrates in instant coffee (C), and total carbohydrates in instant coffee (D); using the modified AOAC official method 995.13 (T = 15 °C).

Download Application Note 280: Carbohydrate in Coffee: AOAC Method 995.13 vs a New Fast Ion Chromatography Method

Coffee: Carbohydrates

		Peaks:	
Column:	Dionex CarboPac PA1 Analytical (4 × 250 mm), Dionex CarboPac PA1 Guard (4 × 50)		1. Mannitol 2. Fucose 3. Rhamnose 4. Arabinose 5. Galactose 6. Glucose 7. Sucrose 8. Fructose 9. Ribose
Flow:	1.0 mL/min		
Temperature:	25 °C		
Injection Volume:	10 µL		
Eluent:	10 mM NaOH 0–6 min DI water 6–50 min 300 mM NaOH from 50–65 min DI water from 65-80 min (re-equilibration)		
Detection:	PAD (Au)		
Postcolumn Reagent:	300 mM Hydroxide		
PCR Flow Rate:	0.6 mL/min		
Traces:	A) Mix of standards B) Green coffee extract		

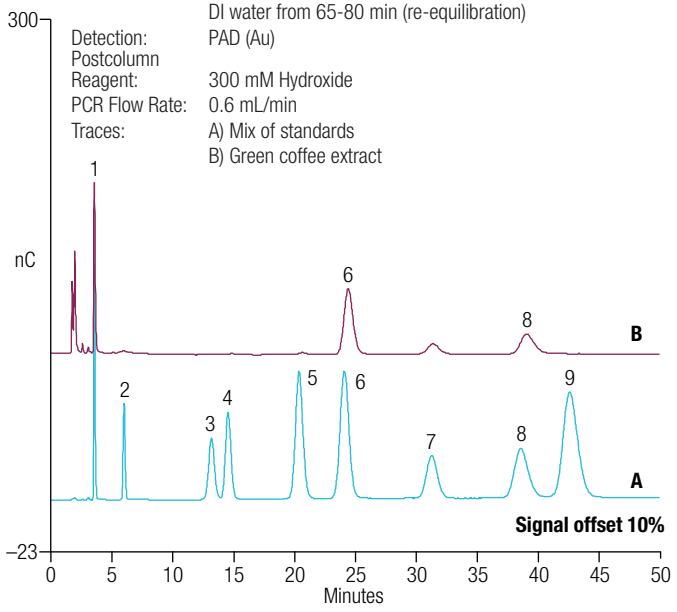


Figure 6-18. Chromatograms of mixed coffee carbohydrate standards (A), free carbohydrates extract from green coffee beans (B); using the modified AOAC official method 995.13 (10 mM hydroxide for 6 min, and xylose and mannose not included in mix of standards).

		Peaks:	
Column:	Dionex CarboPac PA1 Analytical (4 × 250 mm), Dionex CarboPac PA1 Guard (4 × 50)		1. Mannitol 2. Fucose 3. Rhamnose 4. Arabinose 5. Galactose 6. Glucose 7. Xylose 8. Mannose 9. Fructose 10. Ribose
Flow:	1.0 mL/min		
Temperature:	25 °C		
Injection Volume:	10 µL		
Eluent:	10 mM NaOH 0–6 min, DI water 6–50 min 300 mM NaOH from 50–65 min, DI water from 65–80 min (re-equilibration)		
Detection:	PAD (Au)		
Postcolumn Reagent:	300 mM Hydroxide		
PCR Flow Rate:	0.6 mL/min		
Traces:	A) Free carbohydrates extract B) Total carbohydrates extract C) Mix of standards		

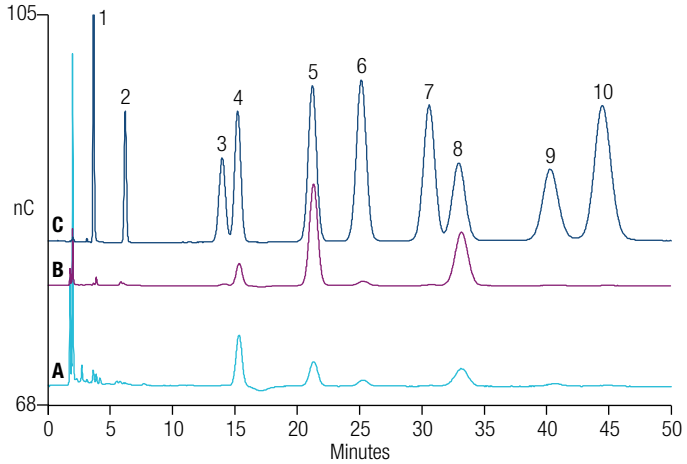


Figure 6-19. Chromatograms of free carbohydrates extract from tnstant coffee (A), total carbohydrates extract from instant coffee (B), and mixed carbohydrate standards (C); using the modified AOAC official method 995.13

Thermo SCIENTIFIC

Coffee: Chlorogenic Acid Esters in Coffee Bean Extracts

One rich source of phenolic antioxidant compounds is coffee, where a range of chlorogenic acids is found. For people who consume coffee beverages regularly, whether prepared from soluble powders or freshly brewed, daily intakes of 500 mg or even more of chlorogenic acids are easily achieved. Chlorogenic acids are a family of esters formed between quinic acid and certain trans-cinnamic acids, most commonly caffeic, p-coumaric and ferulic. As many as 45 of these chlorogenic acids have been reported in coffee. Thus quantification of individual compounds by absorbance detection requires good chromatographic separation.

Application Note 20610 describes an HPLC method using a solid core HPLC column and UV detection for the measurement of twelve chlorogenic acids.

Conditions for Figures 6-20 and 6-21

Instrumentation:	Thermo Scientific™ Accela™ HPLC system
Column 1:	Fully porous C18, 4 µm, 250 × 2.0 mm
Column 2:	Accucore RP-MS, 2.6 µm, 150 × 3.0 mm
Mobile Phase:	A: 0.1% formic acid in water
	B: 0.1% formic acid in acetonitrile
Gradient (Column 1):	Time (min) % B
	0 5
	20 10
	60 35
Flow:	200 µL/min
Gradient (Column 2):	Time (min) % B
	0 2
	8 7
	15 50
Flow:	700 µL/min
Backpressure:	Approx. 200 bar (at starting conditions for both columns)
Column Temperature:	40 °C
Injection Volume:	5 µL
Detection:	UV absorbance detection at 325 nm
Sample Preparation	Soluble coffee extract (Futureceuticals Inc. USA) in water/methanol (90:10 v/v)
Software:	Thermo Scientific Xcalibur v1.3

Download Application Note 20610: Fast Analysis of Coffee Bean Extracts Using a Solid Core HPLC Column

Coffee: Chlorogenic Acid Esters in Coffee Bean Extracts

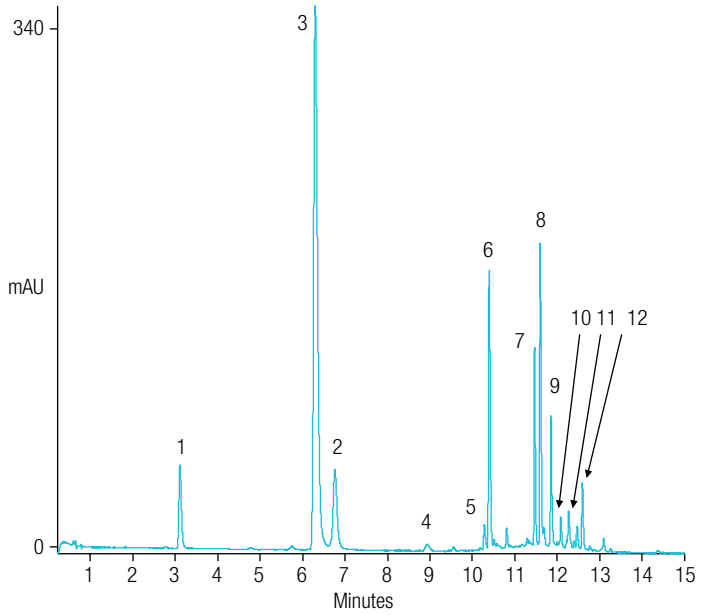


Figure 6-20. Analysis of a coffee bean extract using a 60 minute gradient on a fully porous C18 HPLC column (4 µm particle size, 250 × 2 mm).

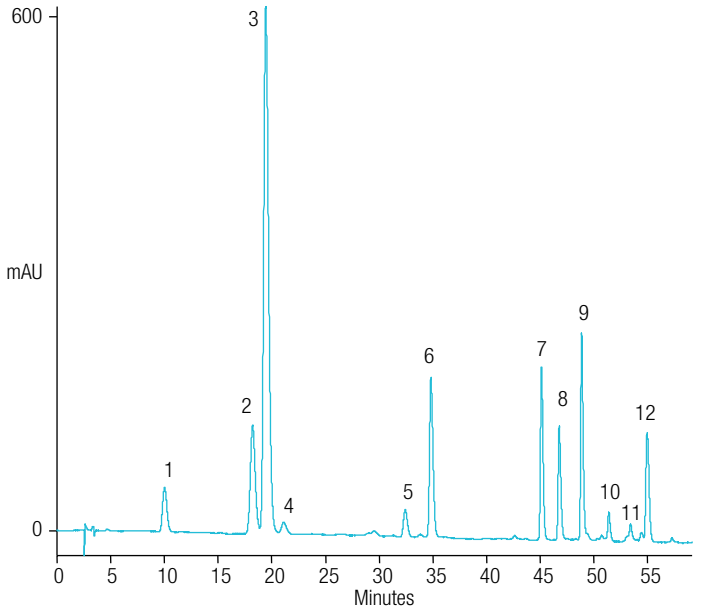


Figure 6-21. Analysis of a coffee bean extract using a 15 minute gradient on a solid core Accucore RP-MS HPLC column (2.6 µm particle size, 150 × 3.0 mm) .

Table 6-1a. Peak numbers and identities of compounds in coffee extracts.

Peak Number	Compound	Peak Number	Compound
1	3-O-Caffeoylquinic acid	**7**	3,4-O-Dicaffeoylquinic acid
2	4-O-Caffeoylquinic acid	**8**	3,5-O-Dicaffeoylquinic acid
3	5-O-Caffeoylquinic acid	**9**	4,5-O-Dicaffeoylquinic acid
4	3-O-Feruloylquinic acid	**10**	3-O-Feruloyl-4-O-caffeoylquinic acid
5	4-O-Feruloylquinic acid	**11**	3-O-Caffeoyl-5-O-feruloylquinic acid
6	5-O-Feruloylquinic acid	**12**	4-O-Caffeoyl-5-O-feruloylquinic acid

Thermo SCIENTIFIC

Download Application Note 20610: Fast Analysis of Coffee Bean Extracts Using a Solid Core HPLC Column

Coffee: Anions and Organic Acids

Although the coffee experience is often highly individualistic, the characteristic aroma, acidity, and flavor of a coffee are attributed to the inorganic anions, organic acids, chlorogenic acid, and monosaccharides content. Organic acids—such as malic, quinic, acetic, formic, and citric—provide much of the acidity associated with coffee.

The organic acid content and profile are characteristic of the coffee type, coffee fruit (cherry) maturity, and extent of roasting. Quinate is present at high concentrations of 5–16% in beans from immature cherries, whereas malate concentrations are higher and quinate concentrations are lower in beans from mature cherries. Higher malate and quinate concentrations are characteristic of Arabica rather than Robusta coffee beans. Organic acids are volatile compounds and thus the concentrations are reduced during the roasting process. Therefore, organic acid determinations are needed to characterize the Arabica bean maturity and extent of roasting. Additionally, these organic acid determinations can profile Robusta and Arabica coffees to determine Robusta content due to blending or adulteration.

Application Brief 135 describes the simultaneous measurement of inorganic anions and organic acid anions in caffeinated and decaffeinated brewed coffee samples using anion-exchange capillary chromatography with suppressed conductivity detection.

Column:	Thermo Scientific™ Dionex™ IonSwift™ MAX-100 guard, MAX-100 capillary, 0.25 × 250 mm
Flow:	12 µL/min
Column Temp.:	30 °C
Injection Volume:	0.4 µL
Eluent Source:	Dionex EGC-KOH capillary
Gradient:	0.1 mM KOH from –10 to 4 min, 0.1–2 mM from 4 to 6 min, 2–15 mM from 6 to 12 min, 15–35 mM from 12 to 16 min, 65 mM from 17 to 30 min
Detection:	Suppressed conductivity, Thermo Scientific™ Dionex™ ACES™ Anion Capillary Electrolytic Suppressor, recycle mode
Sample Prep.:	1:50 dilution

Peaks:

1. Quinate
2. Lactate
3. Acetate
4. Propionate
5. Formate
6. Chloride
7. Bromide
8. Nitrate
9. Glutarate
10. Malate
11. Itaconate
12. Sulfate
13. Fumarate
14. Oxalate
15. Phosphate
16. Citrate
17. Isocitrate

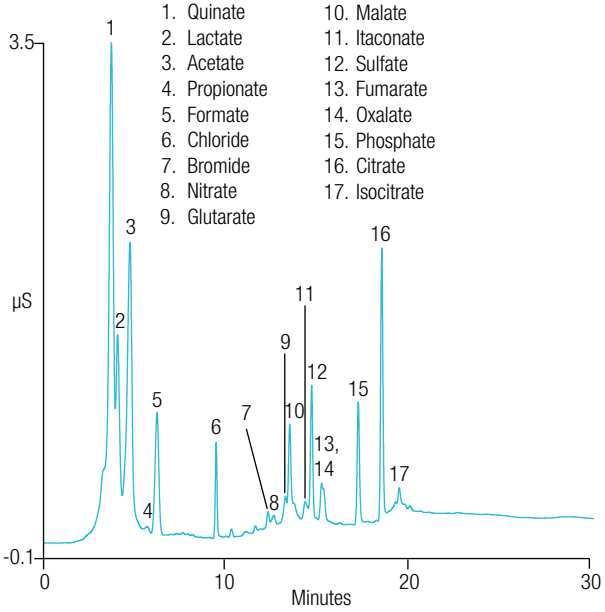


Figure 6-22. Separation of anions in a brewed caffeinated coffee sample by capillary IC on a Dionex IonSwift MAX-100 column.

Download Application Brief 135: Determination of Anions and Organic Acids in Brewed Coffee Samples Using Capillary IC

Coffee: Anions and Organic Acids

Column:	Dionex IonSwift MAX-100 guard, MAX-100 capillary, 0.25 × 250 mm
Flow:	12 µL/min
Column Temp.:	30 °C
Injection Volume:	0.4 µL
Eluent Source:	Dionex EGC-KOH capillary
Gradient:	0.1 mM KOH from –10 to 4 min, 0.1–2 mM from 4 to 6 min, 2–15 mM from 6 to 12 min, 15–35 mM from 12 to 16 min, 65 mM from 17 to 30 min
Detection:	Suppressed conductivity, Dionex ACES, recycle mode
Sample Prep.:	1:50 dilution

Peaks:

1. Quinate
2. Lactate
3. Acetate
4. Propionate
5. Formate
6. Chloride
7. Bromide
8. Nitrate
9. Glutarate
10. Malate
11. Itaconate
12. Sulfate
13. Fumarate
14. Oxalate
15. Phosphate
16. Citrate
17. Isocitrate

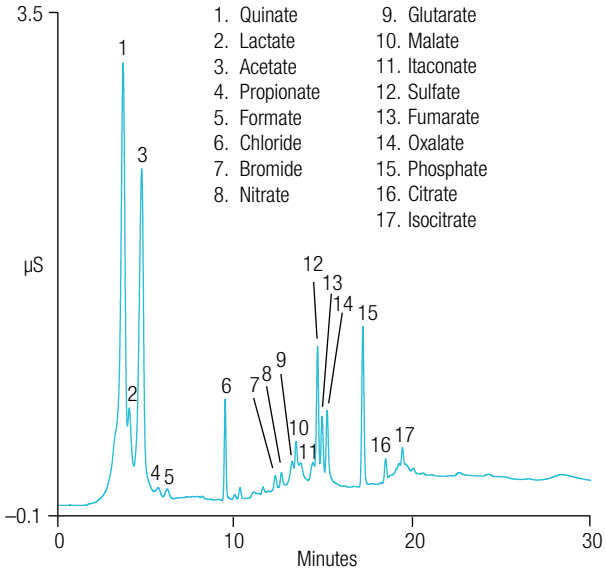


Figure 6-23. Separation of anions in a brewed decaffeinated coffee sample by capillary IC on a Dionex IonSwift MAX-100 column.

Thermo SCIENTIFIC

Table of Contents

Profiling Beverages

Fermentation Broths

Fermentation with yeast, bacteria, or other microorganisms has been used for centuries to produce alcoholic beverages, bread, cheese, yogurt, and feed stock for animals. Fermentation with other microorganisms has more recently been used to produce antibiotics such as penicillin and pharmaceutical compounds, enzymes, amino acids, and organic acids as well as ethanol for fuel or fuel additives.

Thermo SCIENTIFIC

Beer and Wine Fermentation Broths

Fermentation broths are complex mixtures of microorganisms and both organic and inorganic compounds. Ionic compounds, carbohydrates, and amino acids are essential for cellular growth and structure.

For beer and wine, the absence or presence of aldehydes and glycols affects their quality and flavor. Application Note 188 describes the routine measurement of alcohols and glycols by ion exclusion chromatography and pulsed amperometric detection (PAD).

Trivia Question

Q: Do you know how many grapes it takes to make a bottle of wine?

A: It takes approximately 2 1/2 pounds of grapes to make one bottle of wine.

		Peaks:	
Column:	Dionex IonPac ICE-AS1 (4 mm)	1. Exclusion volume	— µM
Eluent:	100 mM methanesulfonic acid	2–3. Unknown	—
Flow:	0.2 mL/min	4. Glycerol	—
Temperature:	30 °C	5–6. Unknown	—
Injection Volume:	10 µL	7. Ethanol	26
Detection:	PAD, Pt (disposable)	8. Unknown	—
Sample Prep:	Supernatant from heat-quenched, centrifuged broth, diluted 300-fold		

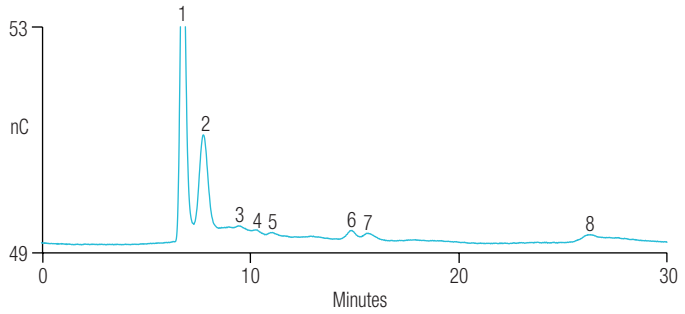


Figure 6-24. American wheat *S. cerevisiae* fermentation broth.

Table 6-2. Waveform for Figures 6-22–6-24.

Time (sec)	Potential vs Ag/AgCl (V)	Gain Region	Integration	Ramp
0.00	+ 0.30	Off	Off	Ramp
0.31	+ 0.30	On	Off	Ramp
0.32	+ 1.15	On	Off	Ramp
0.64	+ 1.15	On	On (Start)	Ramp
0.66	+ 1.15	On	Off (End)	Ramp
0.67	- 0.30	On	Off	Ramp
1.06	- 0.30	Off	Off	Ramp
1.07	+ 0.30	Off	Off	Ramp

Beer and Wine Fermentation Broths

Organic acids, alditols (sugar alcohols), glycols, alcohols, and other compounds are metabolic byproducts. To optimize growth and yields, it is crucial to monitor fermentation broths for both cellular fuel sources as well as metabolic byproducts. Many of these carbohydrates, amino acids, anions, and organic acids have been successfully monitored in fermentation media and broths using ion chromatography (as shown in Application Notes 122, 123 and 150).

		Peaks:		
Column:	Dionex IonPac ICE-AS1 (4 mm)			
Flow:	0.2 mL/min		1. Exclusion volume	— µM
Temperature:	30 °C		2. Unknown	—
Injection Volume:	10 µL		3. Glycerol	39.9
Eluent:	100 mM methanesulfonic acid		4–6. Unknown	—
Detection:	PAD, Pt (disposable)		7. Ethanol	2671
Sample:	Supernatant of degassed and centrifuged sample			

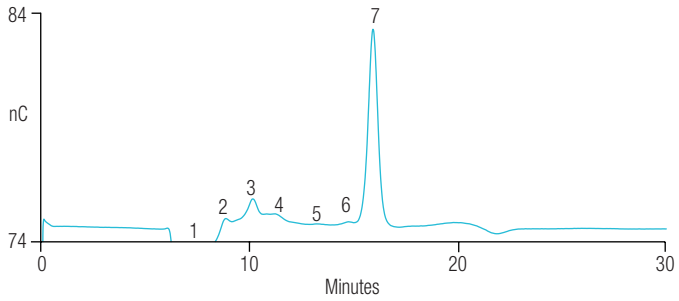


Figure 6-25. 40 µM glycerol and 400 µM ethanol spiked into a 400-fold dilution of German lager.

		Peaks:		
Column:	Dionex IonPac ICE-AS1 (4 mm)			
Flow:	0.2 mL/min		1. Exclusion volume	— µM
Temperature:	30 °C		2-4. Unknown	—
Injection Volume:	10 µL		5. Glycerol	399
Eluent:	100 mM methanesulfonic acid		6. Unknown	—
Detection:	PAD, Pt (disposable)		7. Ethanol	6799
Sample:	Supernatant of centrifuged sample, 400-fold dilution			

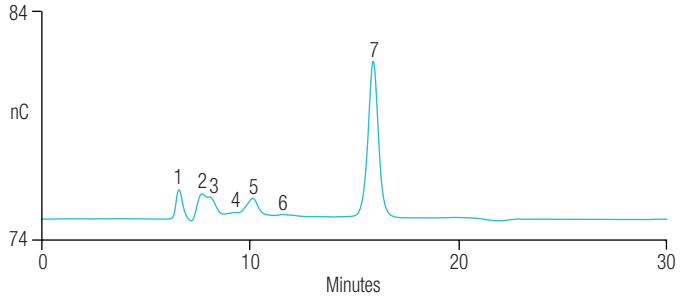


Figure 6-26. Glycerol and ethanol in Chardonnay.

Did You Know?

The difference between champagne and sparkling wine is all in where the wine is made. If the sparkling wine is made in an area in France known as Champagne, then it can be called champagne. If not, it is just sparkling wine.

Download Application Note 122: The Determination of Carbohydrates, Alcohols, and Glycols in Fermentation Broths
Download Application Note 123: Determination of Inorganic Anions and Organic Acids in Fermentation Broths
Download Application Note 150: Determination of Amino Acids in Cell Cultures and Fermentation Broths

Thermo SCIENTIFIC

Yeast and Bacterial Fermentation Broths

Application Note 123 describes the use of two different anion-exchange columns, with suppressed conductivity detection, to determine common organic and inorganic anions in yeast and bacterial fermentation broths. The yeast *Saccharomyces cerevisiae* in yeast extract peptone dextrose (YPD) broth and the bacteria *Escherichia coli* in Luria-Bertani (LB) broth are common fermentation broth cultures and represent eukaryotic and prokaryotic systems. Both fermentation broth cultures are complex and contain undefined media ingredients, and thus are a great challenge for most separation and detection technologies. These formulations also contain carbohydrates, sugar alcohols, alcohols, and glycols that have been analyzed using the Dionex CarboPac PA1, PA10, and MA1 anion-exchange columns with pulsed amperometric detection.

Column:	Dionex IonPac AS11, AG11
Flow:	2.0 mL/min
Temperature:	Ambient
Injection Volume:	10 µL
Eluent:	0.5 mM sodium hydroxide, hold for 2.5 min; 0.5–5 mM sodium hydroxide in 3.5 min; 5–38 mM sodium hydroxide in 12 min.
Sample:	10 mg/L each analyte

Peaks:
1. Lactate
2. Acetate
3. Propionate
4. Formate
5. 2-Keto-d-Gluconate
6. Pyruvate
7. Valerate
8. Monochloroacetate
9. Bromate
10. Chloride
11. Phenylacetate
12. Bromide
13. Nitrate
14. Malate
15. Methylmalonate
16. Carbonate
17. Malonate
18. Maleate
19. Sulfate
20. Oxalate
21. Trichloroacetate
22. Phosphate
23. Citrate
24. Isocitrate
25. Pyrophosphate

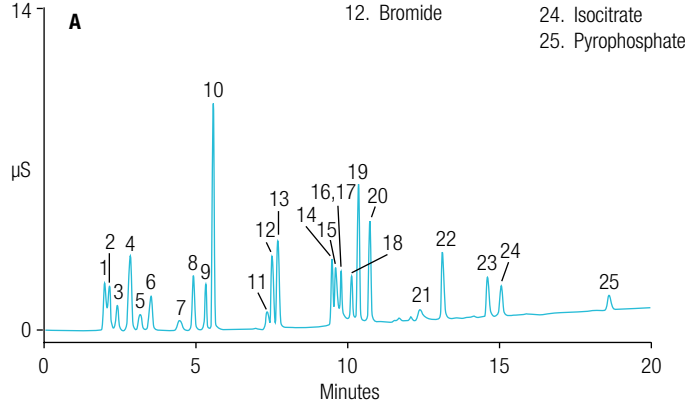


Figure 6-27. Common organic and inorganic anions found in fermentation broths analyzed on the Dionex IonPac AS11 column with suppressed conductivity.

Column:	Dionex IonPac AS11-HC, AG11-HC
Flow:	1.5 mL/min
Temperature:	30 °C
Injection Volume:	10 µL
Eluent:	1 mM sodium hydroxide, hold for 8 min; 1–15 mM sodium hydroxide in 10 min; 15–30 mM sodium hydroxide in 10 min; 30–60 mM sodium hydroxide in 10 min; 60 mM sodium hydroxide, hold for 2 min.
Sample:	10 mg/L each analyte
Peaks:	See Figure 6-29

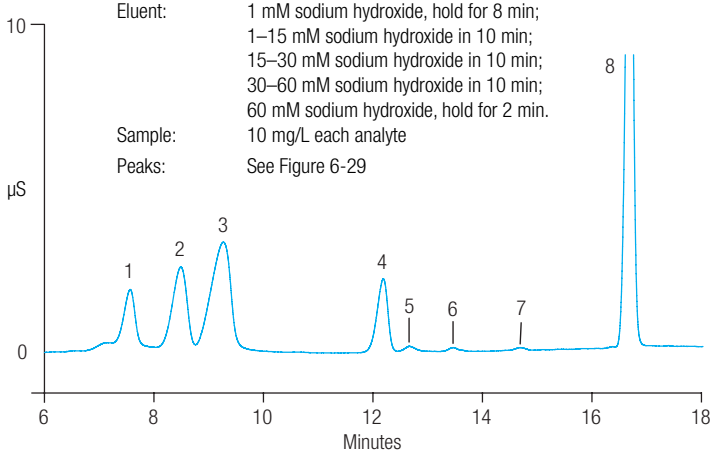


Figure 6-28. Common organic and inorganic anions found in fermentation broths analyzed on the Dionex IonPac AS11-HC column with suppressed conductivity.

Yeast and Bacterial Fermentation Broths

Column:	Dionex IonPac AS11, AG11
Eluent:	0.5 mM sodium hydroxide, hold for 2.5 min; 0.5–5 mM sodium hydroxide in 3.5 min; 5–38 mM sodium hydroxide in 12 min
Flow:	2.0 mL/min
Temperature:	Ambient
Injection Volume:	10 µL
Detection:	Suppressed conductivity, Dionex ASRS suppressor AutoSuppression recycle mode
Peaks:	1. Unknown 2. Lactate 3. Acetate/Glycolate 4. Formate 5. Butyrate 6. Pyruvate/Isovalerate 7. Valerate 8. Chloride

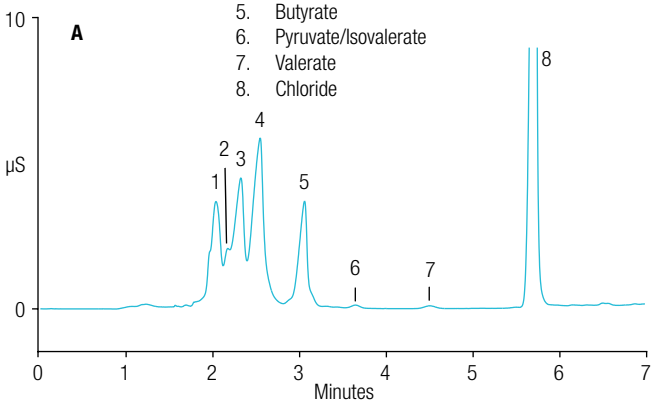


Figure 6-29. *S. cerevisiae* fermentation broth culture (10-fold dilution) using the Dionex IonPac AS11 column at 24 h of incubation.

Column:	Dionex IonPac AS11-HC, AG11-HC
Flow:	1.5 mL/min
Temperature:	30 °C
Injection Volume:	10 µL
Eluent:	1 mM sodium hydroxide, hold for 8 min; 1–15 mM sodium hydroxide in 10 min; 15–30 mM sodium hydroxide in 10 min; 30–60 mM sodium hydroxide in 10 min; 60 mM sodium hydroxide, hold for 2 min.
Sample:	10 mg/L each analyte
Peaks:	See Figure 6-29

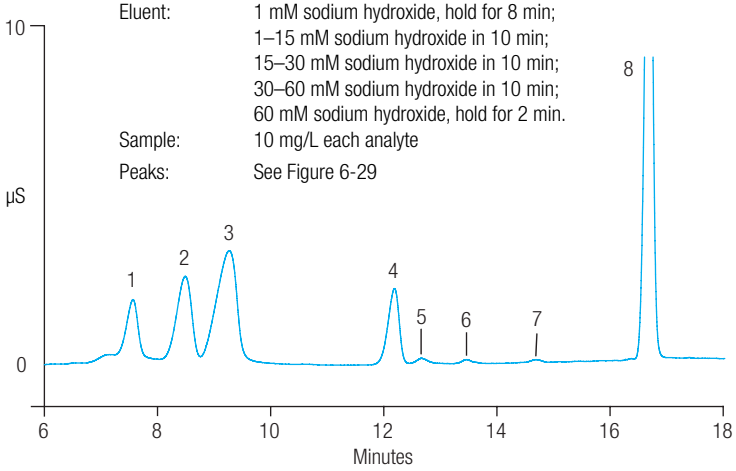


Figure 6-30. *S. cerevisiae* fermentation broth culture (10-fold dilution) using the Dionex IonPac AS11-HC column at 24 h of incubation.

Thermo SCIENTIFIC

Yeast and Bacterial Fermentation Broths

Column:	Dionex IonPac AS11/AG11
Flow:	2.0 mL/min
Injection Volume:	10 µL
Eluent:	0.5 mM sodium hydroxide, hold for 2.5 min; 0.5–5mM sodium hydroxide in 3.5 min; 5–38 mM sodium hydroxide in 12 min.
Detection:	Suppressed conductivity, Dionex ASRS suppressor, AutoSuppression recycle mode
Sample:	*E. coli* culture supernatant, diluted 10-fold

Peaks:

1. Unknown
2. Unknown
3. Unknown
4. Lactate
5. Acetate
6. Propionate
7. Formate
8. Valerate
9. Chloride
10. Unknown
11. Phenylacetate
12. Bromide
13. Nitrate/ 5-Keto-d-Gluconate
14. Unknown
15. Unknown
16. Malate/Succinate
17. Malonate/Carbonate
18. Sulfate
19. Fumarate/Oxalate
20. Phosphate

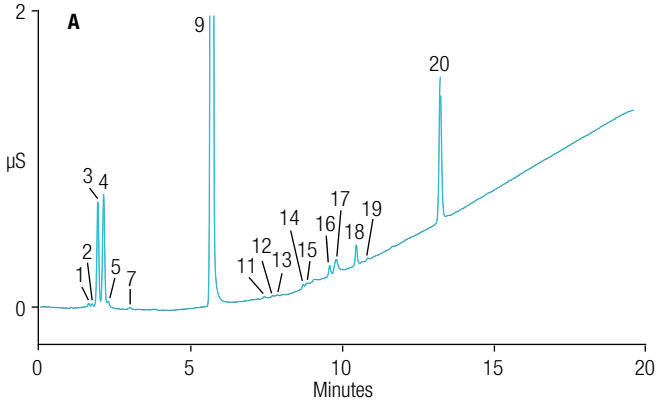


Figure 6-31. *E. coli* fermentation broth culture using the Dionex IonPac AS11 column at 0 h of incubation.

For conditions and peak identifications see Figure 6-34A.

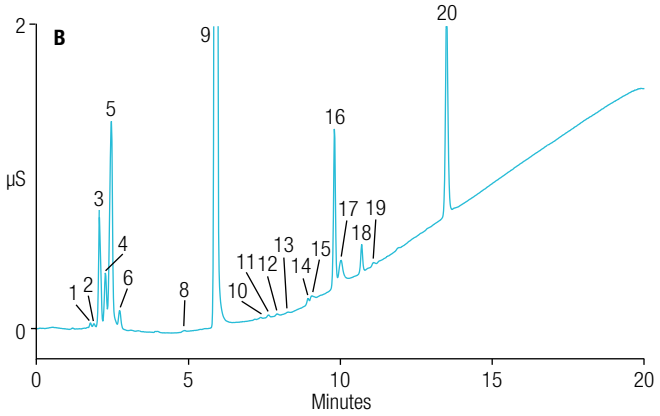


Figure 6-32. *E. coli* fermentation broth culture using the Dionex IonPac AS11 column at 24 h of incubation.

Did You Know?

Before thermometers were invented, brewers would dip a thumb or finger into the mix to find the right temperature for adding yeast. Too cold, and the yeast wouldn't grow. Too hot, and the yeast would die. This thumb in the beer is where "rule of thumb" comes from.

Thermo SCIENTIFIC

Table of Contents

Profiling Beverages

Fruit Juice

Determinations of organic acids in fruit juices are used by the beverage industry for flavor characterization, identification of spoilage, identification of adulteration by a less costly juice, and product labeling

Thermo SCIENTIFIC

Table of Contents

Fruit Juice: Carbohydrates

The measurement of carbohydrates is important for quality control, nutritional labeling, authenticity testing, and production process monitoring because it provides key metrics of product quality and related properties, contamination, or adulteration.

Application Brief 127 describes the use of high-performance anion-exchange chromatography (HPAE) coupled with pulsed amperometric detection (PAD) for direct quantification of non-derivatized carbohydrates with minimal sample preparation. This approach also resolves most carbohydrates from sugar alcohols and organic acids, while not detecting sodium chloride commonly present in fruit juices.

Column:	Dionex CarboPac PA20, 0.4 × 150 mm
Flow:	10 µL/min
Temperature:	30 °C
Injection Volume:	0.40 µL
Eluent:	50 mM potassium hydroxide (EG)
Detection:	PAD, 4–potential carbohydrate, Au
Ref. Electrode:	PdH
Gasket Thickness:	25 µm
Samples:	Juice samples (5000× dilution) Standard (20 µM)

Peaks: 1. Glucose
2. Fructose
3. Sucrose

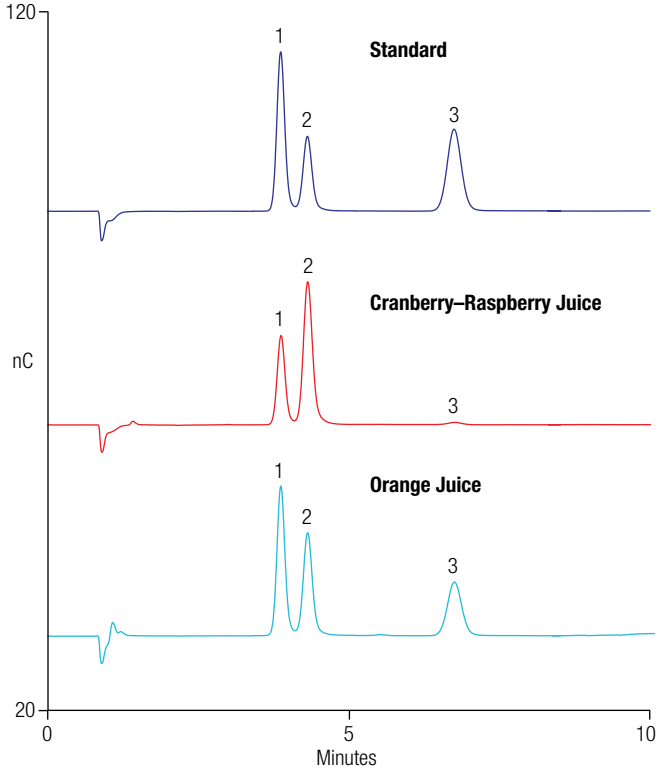


Figure 6-33. Analysis of juices for carbohydrates by capillary HPAE-PAD.

Fruit Juice: Inorganic and Organic Acids

The concentrations, types, and ratios of organic acids are largely responsible for the flavors, tartness, and acidity; therefore, these organic acid analyses are important for delivering a consistent and fresh juice product. Additionally, two common organic acids, acetate and lactate, are caused by biological activity and are, therefore, a good indicator of an old juice that may be too spoiled for consumption.

Application Brief 137 describes the use of capillary ion-exchange columns with suppressed conductivity detection for the measurement of a number of inorganic and organic acids in apple and orange juice samples.

Did You Know?

According to the US Department of Agriculture, Americans consumed over 700,000 metric tons of orange juice in 2013.

Column:	Dionex IonSwift MAX-100 guard, MAX-100, capillary, 0.25 mm
Flow:	15 µL/min
Column Temp.:	30 °C
Injection Volume:	0.4 µL
Eluent Source:	Dionex EGC-KOH capillary cartridge
Gradient:	0.1 mM KOH from -10 to 0.1 min, 0.1–2 mM from 0.1 to 3.3 min, 2–25 mM from 3.3 to 13.3 min, 25–65 mM from 13.3 to 20 min, 65 mM from 20 to 25 min
Detection:	Suppressed conductivity, Dionex ACES suppressor, recycle
Samples:	A: Apple juice, B: Orange juice
Sample Prep.:	1:40 dilution, filter, 0.45 µm

Peaks:	A	B
1. Quinate	6	2 mg/L
2. Glycolate	0.2	—
3. Lactate	5	3
4. Acetate	—	0.1
5. Formate	0.1	0.7
6. Pyruvate	0.3	—
7. Galacturonate	0.4	—
8. Chloride	0.3	1
9. Nitrate	—	0.4
10. Glutarate	—	4
11. Malate	40	25
12. Maleate	—	0.1
13. Sulfate	2	2
14. Oxalate	0.1	4
15. Phosphate	3	7
16. Citrate	0.1	125
17. Isocitrate	—	—
18. *cis*-Aconitate	—	—
19. *trans*-Aconitate	—	—

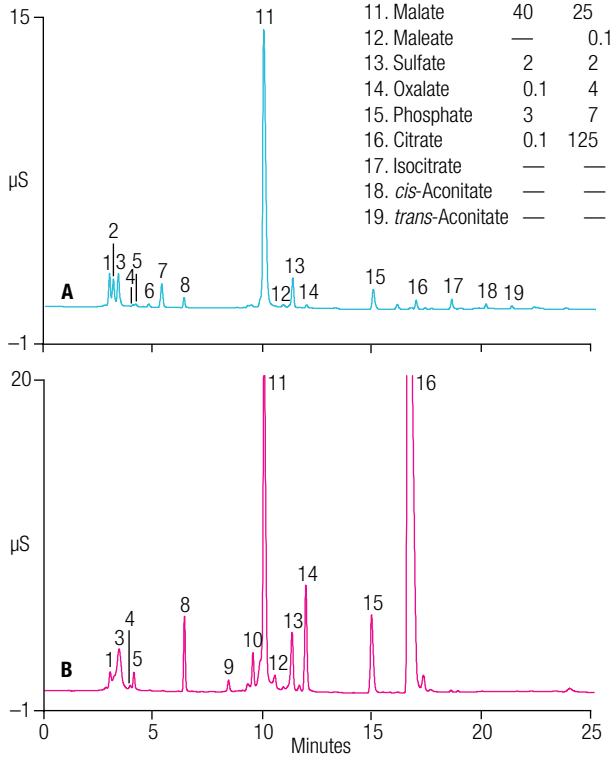


Figure 6-34. Measurement of inorganic anions and organic acids in diluted A) apple juice and B) orange juice samples.

Download Application Brief 137: Determination of Inorganic and Organic Acids in Apple and Orange Juice Samples Using Capillary IC

Fruit Juice: Inorganic and Organic Acids

Table of Contents

Peaks:							
1.	Quinate	55	ppm	9.	Malate	116.0	ppm
2.	Fluoride	1.3		10.	Malonate/Tartrate	190.0	
3.	Lactate	46.2		11.	Maleate	4.0	
4.	Galacturonate	60		12.	Sulfate	22.1	
5.	Chloride	1.2		13.	Oxalate	19.4	
6.	Nitrate	0.6		14.	Phosphate	27.0	
7.	Glutarate	0.7		15.	Citrate	80.0	
8.	Succinate	1.2		16.	Isocitrate	1.8	

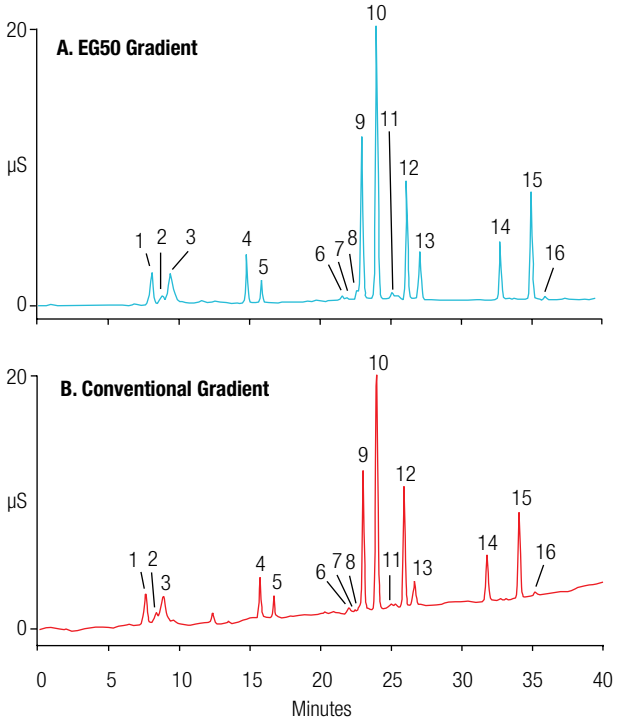


Figure 6-35. Determination of anions and organic acids in grape juice.

Peaks:							
1.	Quinate	34.5	mg/L	10.	Malate	250.1	mg/L
2.	Lactate	14.8		11.	Malonate/Tartrate	0.8	
3.	Glycolate	0.6		12.	Maleate	1.6	
4.	Formate	0.5		13.	Sulfate	1.7	
5.	Pyruvate	1.2		14.	Oxalate	0.5	
6.	Galacturonate	1.5		15.	Phosphate	12.6	
7.	Chloride	0.4		16.	Citrate	6.6	
8.	Nitrate	0.8		17.	Isocitrate	0.4	
9.	Succinate	9.0		18.	Cis-aconitate	0.4	

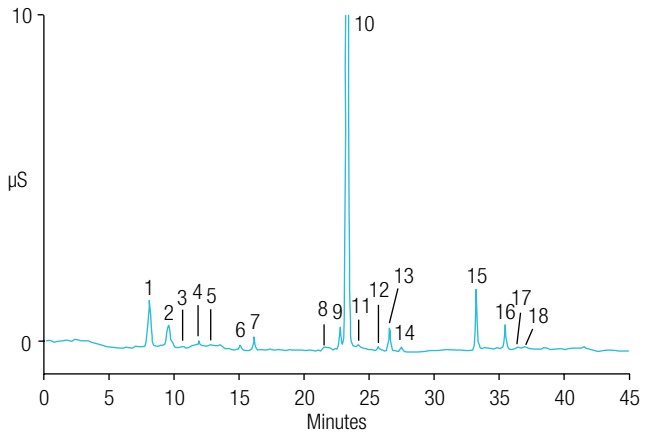


Figure 6-36. Determination of anions and organic acids in apple juice.

Thermo SCIENTIFIC

Fruit Juice: Inorganic and Organic Acids

Peaks:	1.	Quinate	210 mg/L	11.	Succinate	257 mg/L
	2.	Fluoride	<0.1	12.	Unknown	–
	3.	Lactate/Acetate	10	13.	Sulfate	10.3
	4.	Glycolate	2.6	14.	Oxalate	14.8
	5.	Formate	3.7	15.	Phosphate	1.8
	6.	Pyruvate	2.1	16.	Unknown	–
	7.	Unknown	–	17.	Citrate	163
	8.	Galacturonate	16.9	18.	Isocitrate	1.0
	9.	Chloride	2.3	19.	Trans-aconitate	2.7
	10.	Nitrate	<0.1	20.	Unknown	–

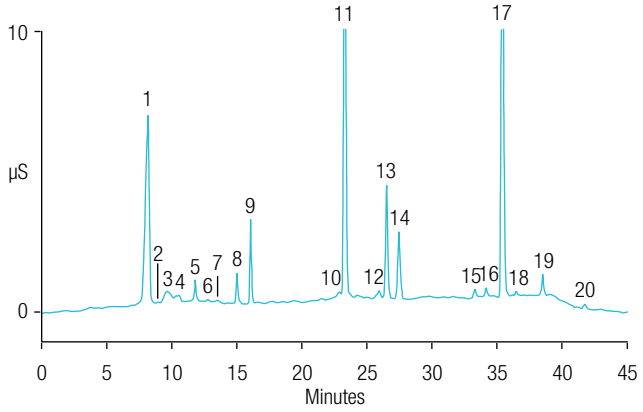


Figure 6-37. Determination of anions and organic acids in cranberry juice cocktail.

Did You Know?

- Cranberry blossoms can last 10 to 12 days, depending on the weather.
- Cranberry bushes thrive in conditions that would not support most plants, including acidic soil with few nutrients and low temperatures.
- The cranberry is one of only a handful of major fruits native to North America. Others include the blueberry and the Concord grape.

Thermo SCIENTIFIC

Fruit Juice: Inorganic and Organic Acids

Table of Contents

Many analytical methods are available to determine organic acids in juices and wines. However, several organic acids have poor UV absorption and therefore lack sufficient sensitivity for detection. In addition, other components commonly present in these types of samples – such as sugars and phenolic compounds – have a much higher UV absorption, which can interfere with the detection of target analytes. In contrast, virtually all carboxylic acids ionize sufficiently; therefore, as describe in Application Note 1068, ion chromatography with suppressed conductivity detection is the technique of choice to separate a large variety of organic acids with inorganic anions and detect them with high sensitivity while minimizing the sugar interferences.

Peaks:							
1. Quinate	5 mg/L	11. Galacturonate	5	21. Tartrate	5
2. Fluoride	1	12. Bromate	10	22. Maleate	10
3. Lactate	5	13. Chloride	2.5	23. Sulfate	5
4. Acetate	5	14. Bromide	5	24. Fumarate	20
5. Glycolate	5	15. Nitrate	5	25. Oxalate	5
6. Propionate	5	16. Glutarate	5	26. Phosphate	10
7. Formate	5	17. Succinate	10	27. Citrate	10
8. Butyrate	5	18. Malate	20	28. Isocitrate	10
9. Pyruvate	5	19. Carbonate	—	29. *cis*-Aconitate	10
10. Valerate	5	20. Malonate	5	30. *trans*-Aconitate	10

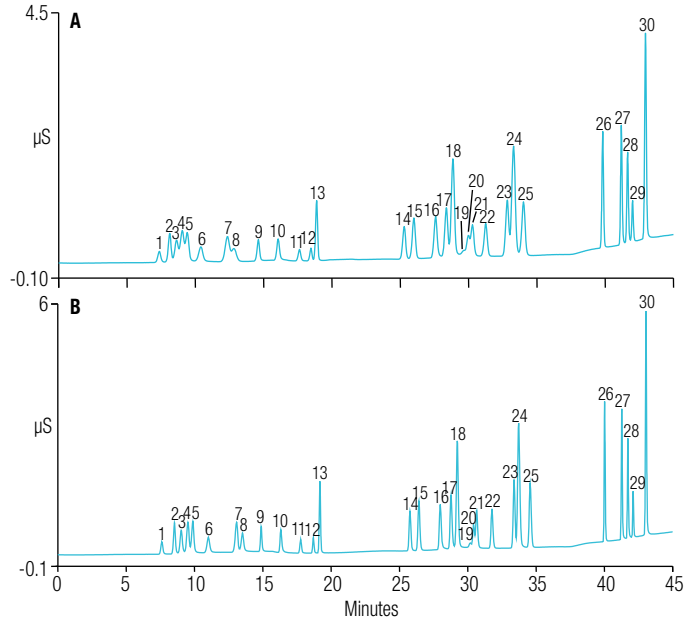


Figure 6-38. Comparison of the resolution of organic and inorganic anion standards on (A) the Dionex IonPac AS11-HC and (B) the Dionex IonPac AS11-HC-4 µm columns.

Download Application Note 1068: Determination of Organic Acids in Fruit Juices and Wines by High-Pressure IC

Fruit Juice: Inorganic and Organic Acids

Peaks:		A		B
1. Quinate	—	mg/L	6.78
2. Fluoride	0.137		0.217
3. Lactate	3.40		18.5
4. Acetate	0.270		0.553
5. Glycolate	0.100		0.312
6. Formate	0.0546		0.0942
7. Butyrate	0.302		0.230
8. Pyruvate	0.0521		0.229
9. Valerate	0.0689		0.0671
10. Galacturonate	3.38		15.6
11. Chloride	22.7		21.1
12. Glutarate	0.591		0.550
13. Succinate	1.44		2.41
14. Malate	40.8		38.2
15. Carbonate	—		—
16. Tartrate	0.127		0.109
17. Sulfate	4.51		4.43
18. Oxalate	2.14		2.31
19. Phosphate	14.4		14.1
20. Citrate	330		265
21. Isocitrate	7.08		6.17
22. *cis*-Aconitate	4.59		1.73
23. *trans*-Aconitate	0.419		0.367

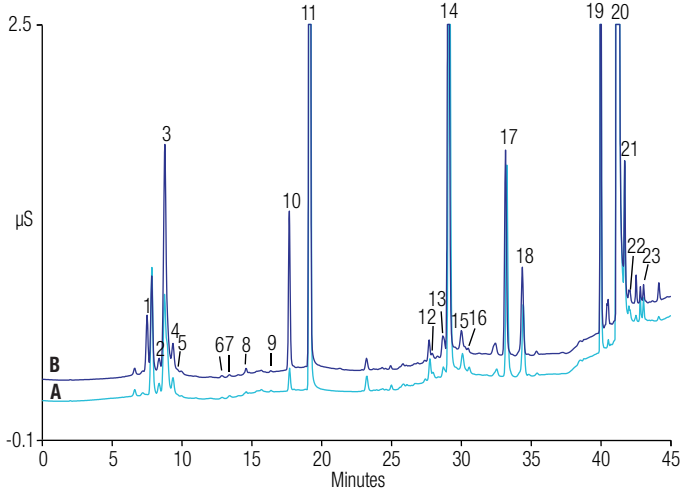


Figure 6-39. (A) Pomegranate juice and (B) pomegranate/blueberry juice analyzed on the Dionex IonPac AS11-HC-4 µm column.

Peaks:		A		B
1. Fluoride	1.05	mg/L	1.36
2. Lactate	3.37		3.23
3. Acetate	0.703		1.21
4. Glycolate	—		0.376
5. Formate	0.128		0.510
6. Butyrate	0.0842		0.295
7. Pyruvate	0.190		0.0847
8. Galacturonate	39.5		71.1
9. Chloride	2.87		2.28
10. Bromide	0.218		0.125
11. Nitrate	0.611		1.72
12. Succinate	1.17		2.17
13. Malate	86.2		141
14. Carbonate	—		—
15. Tartrate	93.5		85.4
16. Maleate	5.90		—
17. Sulfate	14.8		10.1
18. Fumarate	0.345		—
19. Oxalate	7.59		8.74
20. Phosphate	20.6		21.4
21. Citrate	58.4		75.8
22. Isocitrate	2.32		3.30
23. *cis*-Aconitate	0.161		0.900
24. *trans*-Aconitate	0.0995		0.0466

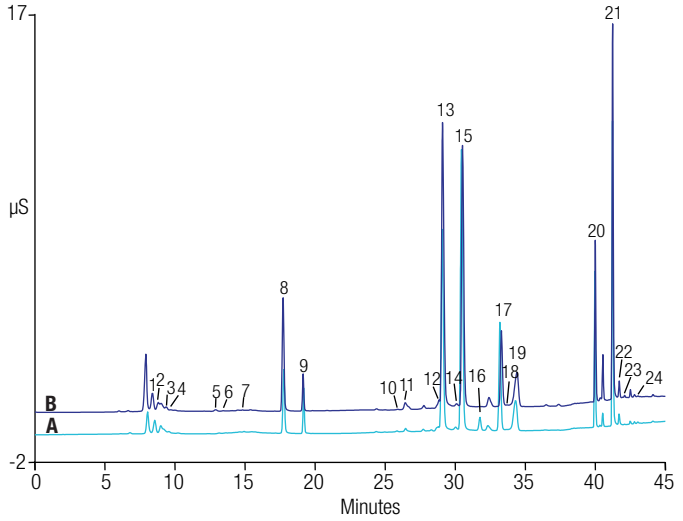


Figure 6-40. (A) White grape juice and (B) grape juice analyzed on the Dionex IonPac AS11-HC-4 µm column.

Fruit Juice: Inorganic and Organic Acids

		A		B			
Peaks:	1. Quinate	17.6	mg/L	17.6	11. Malate	235	461
	2. Fluoride	0.214		0.214	12. Carbonate	—	—
	3. Lactate	4.07		4.07	13. Tartrate	0.335	0.335
	4. Acetate	0.0515		0.0515	14. Sulfate	3.08	3.08
	5. Glycolate	0.258		0.258	15. Oxalate	3.16	3.16
	6. Formate	2.08		2.08	16. Phosphate	8.48	8.48
	7. Pyruvate	0.496		0.496	17. Citrate	2.11	4.28
	8. Galacturonate	83.5		165	18. Isocitrate	0.628	0.628
	9. Chloride	2.19		2.19	19. *cis*-Aconitate	3.00	3.00
	10. Succinate	1.59		1.59	20. *cis*-Aconitate	0.0241	0.0241

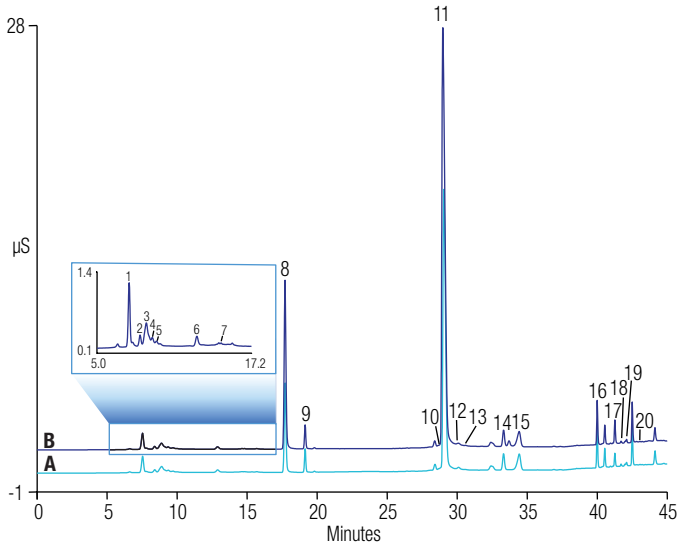


Figure 6-41. (A) Apple juice and (B) spiked apple juice analyzed on the Dionex IonPac AS11-HC-4 µm column.

Thermo SCIENTIFIC

Fruit Juice: Polyphenol Analysis

Table 6-3. Retention time and dominant oxidation channel for the different analytes measured using the gradient-HPLC CoulArray method.

Peak No.	Compound	Retention Time (min)	Dominant EC Channel
1	Gallic acid	2.68	2
2	4-Hydroxybenzyl alcohol	4.44	10
3	p-Aminobenzoic acid	5.08	11
4	3,4-Dihydroxybenzoic acid	5.44	4
5	Gentisic acid	5.57	2
6	2-Hydroxybenzyl alcohol	7.57	10
7	Chlorogenic acid	8.64	2
8	4-Hydroxybenzoic acid	8.71	13
9	p-Hydroxyphenyl acetic acid	9.05	10
10	Catechin	9.57	2
11	Vanillic acid	10.16	8
12	4-Hydroxybenzaldehyde	10.52	13
13	Syringic acid	10.66	6
14	Caffeic acid	11.13	2
15	Vanillin	12.27	9
16	Syringealdehyde	12.95	7
17	Umbelliferone	14.1	11
18	p-Coumaric acid	15	9
19	Sinapic acid	15.78	5
20	Salicylic acid	15.85	13
21	Ferulic acid	16.28	6
22	Ethyl vanillin	17.6	9
23	4-Hydroxycoumarin	20.1	16
24	Hesperidin	20.28	7
25	Naringin	20.4	11
26	Rosemarinic acid	21.34	2
27	Fisetin	22.77	2
28	Myricetin	23.5	1
29	Luteolin	26.3	3
30	Quercetin	26.7	2
31	Kaempferol	29	2
32	Isorhamnetin	29.15	2
33	Eugenol	29.2	6
34	Cavacrol	32.3	9
35	Thymol	32.6	8
36	Carnosol	34.5	5
37	Carnosic acid	36.37	4

Pump:	UltiMate 3000 LPG-3400BM with Solvent Rack SR-3000
Autosampler:	UltiMate 3000 WPS-3000TBSL
Analytical Column:	Acclaim 120, C18, 3 × 150 mm, 3 µm
Flow:	0.65 mL/min
Injection Volume:	10 or 20 µL
Mobile Phase A:	20 mM Monobasic sodium phosphate, 3% acetonitrile, 0.2% tetrahydrofuran, pH 3.35
Mobile Phase B:	20 mM Monobasic sodium phosphate, 50% acetonitrile, 10% Tetrahydrofuran, pH 3.45
Mobile Phase C:	90% Methanol
Gradient:	0-2 min: 2%B/3%C.; 30 min: 97%B/3%C; 45 min 97%B/3%C. Curve 7
EC Detector:	CoulArray Detector with Thermal Organizer Module
EC Parameters:	16-channel array from 0 to +900 mV in +60 mV increments
Peaks:	See Table 6-2

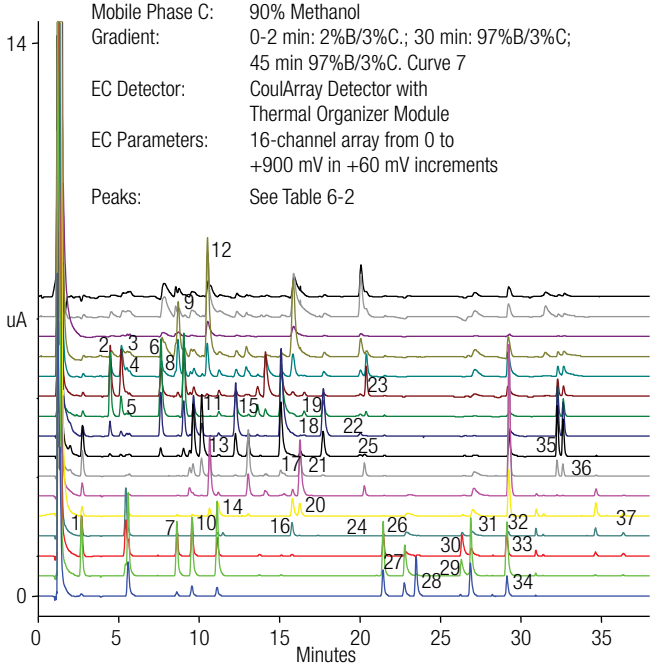


Figure 6-42. Gradient HPLC with coulometric electrochemical array detection.

Download Application Note 1063: Targeted Analyses of Secondary Metabolites in Herbs, Spices, and Beverages Using a Novel Spectro-Electro Array Platform

Download Application Note 1064: Product Authentication and Adulteration Determination Using a Novel Spectro-Electro Array Platform

Infant Formula

Infant formula is a mixture of nutrients and other components designed to roughly mimic human mother's milk at approximately one to three months post partum. There can be significant differences in the nutrient content between commercial products. Infant formula is usually prepared for bottle-feeding or cup-feeding from powder (mixed with water) or liquid (with or without additional water).

Thermo SCIENTIFIC

Infant Formula: Choline

Recent research indicates that choline plays an important role in cardiovascular and liver health and in reproduction and development. Choline may even help improve memory and physical performance. Milk, eggs, organ meats, and other meats are good sources of choline, whereas grains, fruits, and vegetables are poor sources. Choline is essential to proper metabolism, and is therefore often added to vitamin formulations, animal feeds, infant formulas, and sports drinks. It is usually added to these products as the bitartrate or chloride salt and supplied as a solution for oral administration.

Application Update 189 describes methods for extraction of free and bound choline from dry milk and infant formula and its determination in the mg/L range by ion chromatography. The method also allows mineral ions (Na^+, K^+, Mg^{2+}, Ca^{2+}) to be determined simultaneously with choline.

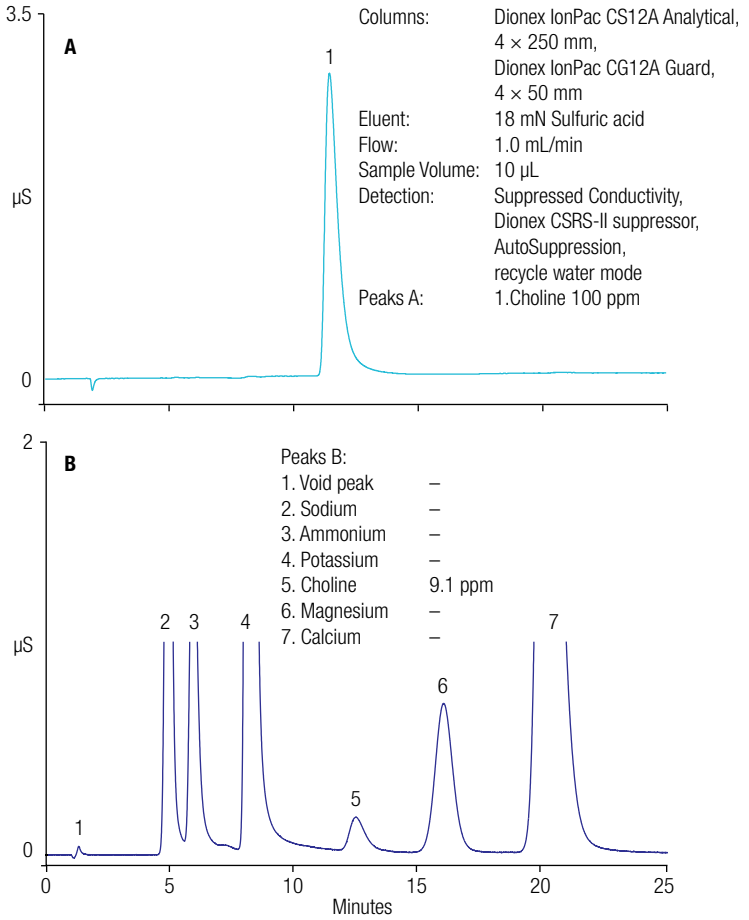


Figure 6-43. Determination of choline in dry milk and infant formula: (A) 100 ppm choline standard and (B) infant formula sample.

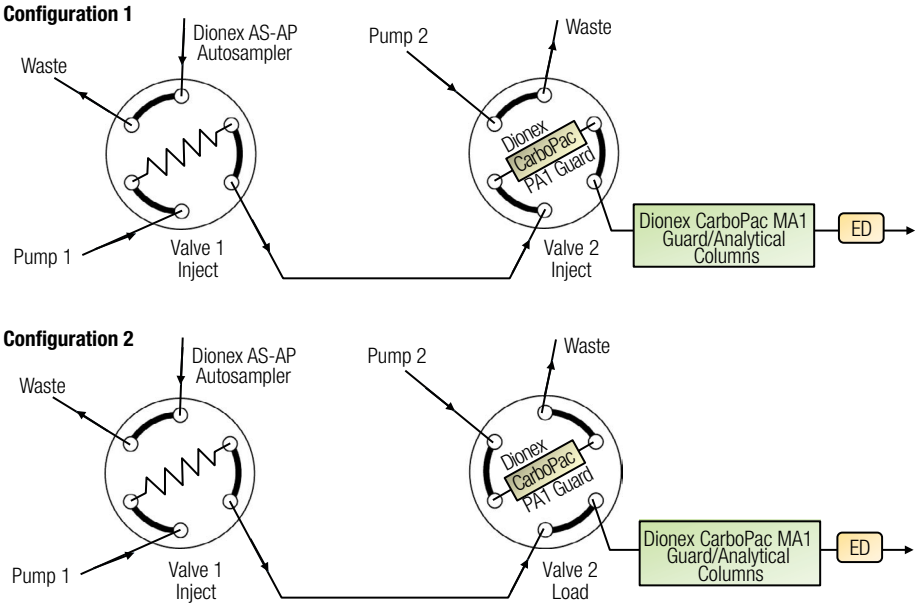
Download Application Update 189: Determination of Choline in Infant Formula and Other Food Samples by IC

Infant Formula: Myo-Inositol Free and Bound as Phosphatidyl-inositol

Myo-inositol is one of the most abundant sugars in the body, where it occurs in its free form and as a component of phosphoinositides in cell membranes. It plays an important role in various biological functions, including the regulation of cell osmolality, phosphoinositide-mediated processes of cell signaling, formation of the neural system, and pulmonary surfactant phospholipid production.

To ensure that infant formula and adult nutritionals meet the minimum requirements for myoinositol, simple and fast methods to determine myoinositol content in these food products are needed.

Application Note 1083 evaluates and describes execution of an HPAE-PAD method combined with the column-switching technique described in AOAC Official Method 2011.18. For the determination of myo-inositol bound as phosphatidylinositol, otherwise known as myo-insitol, is released from its bound form using acid hydrolysis prior to chromatographic analysis.



Time (min)	Configuration
0.00	1
1.50	2
11.2	1

Figure 6-44. Valve-switching configurations with time table.

Download Application Note 1083: Determination of Myo-Inositol (Free and Bound as Phosphatidylinositol) in Infant Formula and Adult Nutritionals

Infant Formula: Myo-Inositol Free and Bound as Phosphatidyl-inositol

Dimension 1

Column:	Dionex CarboPac PA1 Guard, 4 × 50 mm
Eluent:	750 mM Sodium Hydroxide (NaOH)
Flow:	0.4 mL/min
Injection Volume:	20 µL
System	
Backpressure:	800–900 psi

Dimension 2

Column:	Dionex CarboPac MA1 Guard, 4 × 50 mm Dionex CarboPac MA1 Analytical, 4 × 250 mm
Flow:	0.4 mL/min
Temperature:	30 °C
Injection Volume:	20 µL
Eluent:	15 mM KOH
Eluent Source:	Dionex EGC 500 KOH Cartridge with Dionex CR-ATC 500 Trap Column
Detection:	PAD, Au on PTFE Disposable Working Electrode
System	
Backpressure:	2800–2900 psi
Background	
Conductance:	28–41 nC
Noise:	~16 pC/min peak-to-peak
Run Time:	25 min

Peak:	A	B	C	D
1. Myo-inositol	1.00	0.904	0.878	0.0681 mg/L

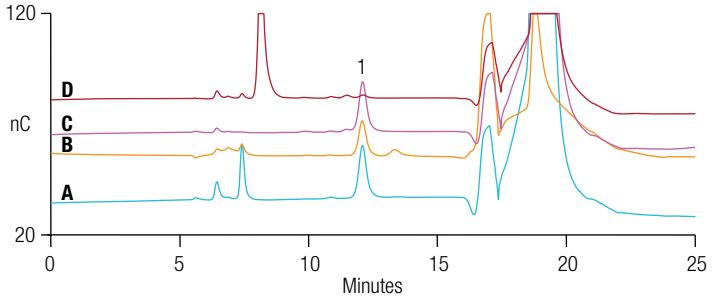


Figure 6-45. Free myo-inositol in (A) SRM 1849, (B) milk-based powdered infant formula, (C) soy-based powdered infant formula, and (D) adult nutritional liquid.

Table 6-4. Waveform for the ED.

Time (s)	Potential (V)	Last Step*	Ramp*	Gain Region*	Integration
0.00	0.1	Off	On	Off	Off
0.20	0.1	Off	On	On	On
0.40	0.1	Off	On	Off	Off
0.41	–2	Off	On	Off	Off
0.42	–2	Off	On	Off	Off
0.43	0.6	Off	On	Off	Off
0.44	–0.1	Off	On	Off	Off
0.50	–0.1	On	On	Off	Off

* Setting required on Dionex ICS-3000/5000/5000+ systems but not used in older Dionex IC systems; reference electrode in AgCl mode

Peaks:	A	B	C	D
1. Glycerol	—	—	—	—
2. Myo-inositol	0.260	0.376	0.301	0.591 mg/L

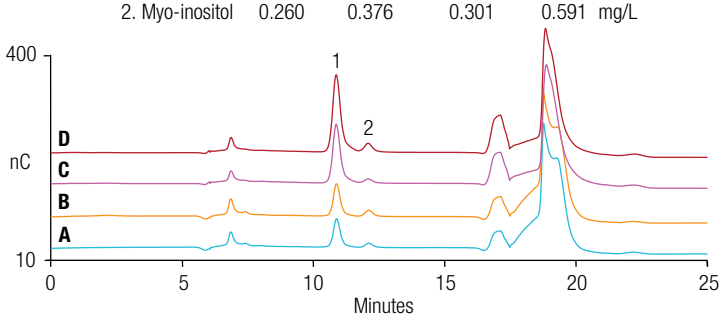


Figure 6-46. Myo-inositol from phosphatidylinositol in (A) soy-based powdered infant formula and (B) soy-based powdered infant formula with 150% spike prepared using Method 1; (C) soy-based powdered infant formula and (D) soy-based powdered infant formula with 50% spike prepared using Method 2. For conditions see Figure 41-B.

Thermo SCIENTIFIC

Infant Formula: Myo-Inositol Free and Bound as Phosphatidyl-inositol

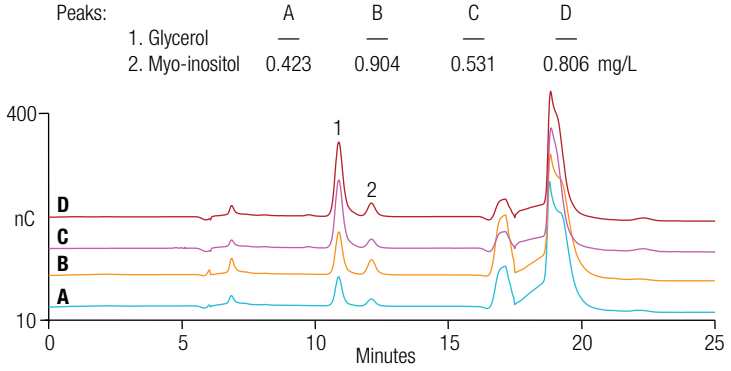


Figure 6-47. Myo-inositol from phosphatidylinositol in (A) milk-based powdered infant formula and (B) milk-based powdered infant formula with 50% spike prepared using Method 1; (C) milk-based powdered infant formula and (D) milk-based powdered infant formula with 100% spike prepared using Method 2. For conditions see Figure 41-B.

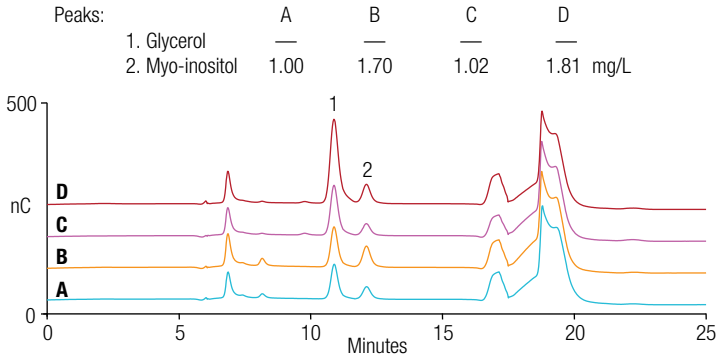


Figure 6-48. Myo-inositol from phosphatidylinositol in (A) adult nutritional liquid and (B) adult nutritional liquid with 100% spike prepared using Method 1; (C) adultnutritional liquid and (D) adult nutritional liquid with 100% spike prepared using Method 2. For conditions see Figure 41-B.

Thermo SCIENTIFIC

Infant Formula: Nucleosides and Nucleotides

The addition of nucleotides to infant formula has beneficial effects on the growth and maturation of the gastrointestinal tract of healthy infants.

Studies show that nucleotides are more abundant in human milk compared to cow milk, hence addition of nucleotides to infant formula may be beneficial.

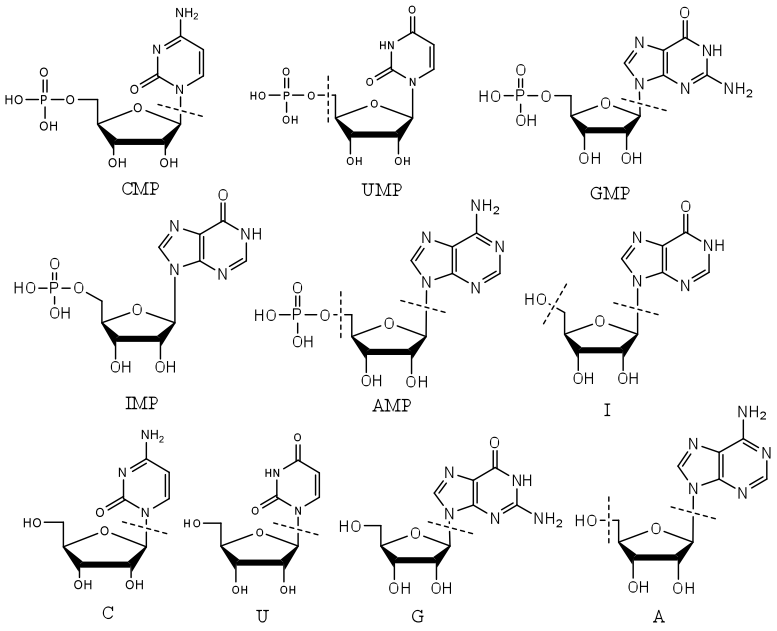


Figure 6-49. Chemical structures of nucleotides found in infant formula.

Column:	Acclaim C30, 2.1 mm × 150 mm, 3 µm (S/N001008, P/N075725			
Flow:	0.4 mL/min			
Injection Volume:	Autosampler 10 µL			
Elution:	A. H_2O			
	B. 100 mmol/L NH_4OAC, pH=5.0			
	C. ACN			
Gradient:	min	%A	%B	%C
	-5	80	20	0
	0	80	20	0
	3	80	20	0
	5.9	70	20	10
	9	42	20	32
	11.9	42	20	32
	12	80	20	0
	15	80	20	0
Detection:	DAD: 260 nm			

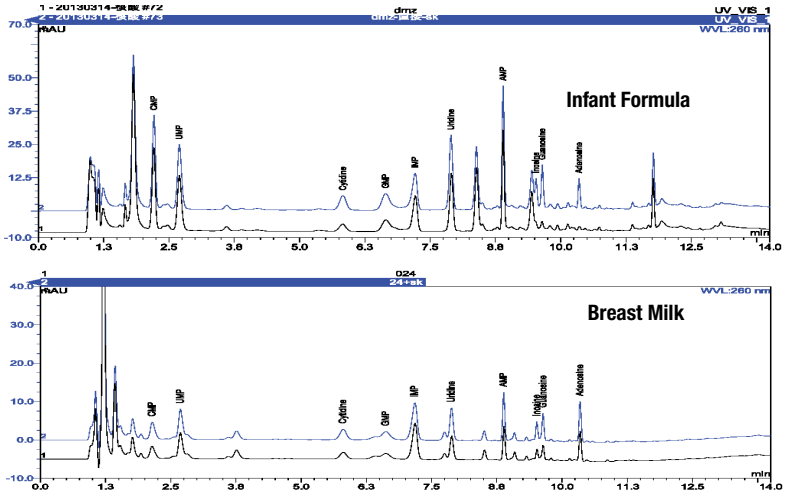


Figure 6-50. Measurement of nucleosides and nucleotides in infant formula and breast milk using gradient HPLC with UV detection. Black traces, sample; blue traces, standard spiked sample.

Thermo SCIENTIFIC

Table of Contents

Profiling Beverages

Black tea

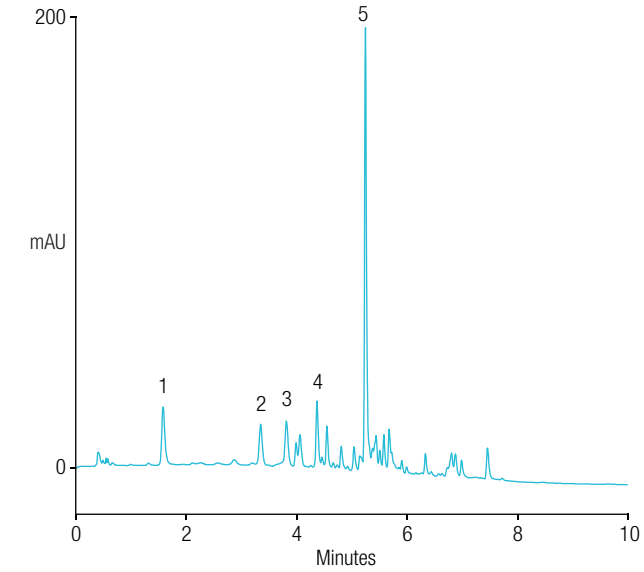
Tea

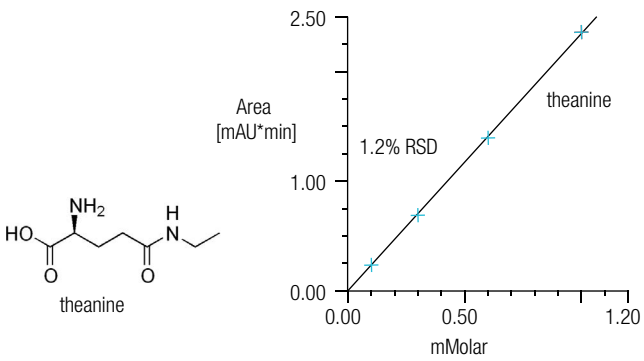
Tea consumption has become increasingly popular, and it is currently one of the most consumed non-alcoholic drinks worldwide. There are four major varieties of teas: white, green, oolong, and black. Although all teas are derived from the same *Camellia sinensis* plant, the processing methods for each tea are different.

Thermo SCIENTIFIC

Tea: Amino Acids

Amino acids, especially glutamate, contribute to the savory "umami" flavor to tea. The most abundant amino acid in green tea is theanine, or *N*′-ethylglutamine. This unusual amino acid is noted for its mild relaxing effect. The amino acids are analyzed by automated precolumn derivatization with o-phthalaldehyde and *N,N*-dimethylamino-ethanethiol.





Column:	Acclaim RSLC PolarAdvantage, 2.2 µm
Dimensions:	3.0 × 50 mm
Flow:	0.60 mL/min
Temperature:	30 °C
Injection Volume:	0.5 µL, automated precolumn derivatization
Mobile Phases:	A: 5 mM citric acid + 20 mM potassium citrate B: Methanol C: Acetonitrile

Gradient Time (min):	-5.0	0.0	1.0	8.0	10.0
%A	90	90	90	35	35
%B	10	10	10	10	10
%B	0	0	0	55	55

Detection:	UV at 330 nm
Sample Preparation:	Extract 200 mg of green tea leaves in 5.0 mL of 100 mM acetic acid at 80 °C for 15 min
Peaks:	1. Aspartate 2. Glutamate 3. Asparagine 4. Glutamine 5. Theanine

Automated Derivatization Conditions

Reagent A:	5 mg/mL *o*-Phthalaldehyde in 0.5 M potassium borate buffer, pH 10.4
Reagent B:	10 mg/mL *N,N*-Dimethylaminoethanethiol hydrochloride in water
Reagent C:	2 M Acetic acid
Program:	Draw 3 µL air, draw 2.5 µL reagent A, draw 0.5 µL sample, wash needle, draw 2.5 µL reagent B, in-needle mixing six times 16 µL, wait 60 s, wash needle, draw 1.5 µL reagent C, mix three times 16 µL, inject.

Figure 6-51. Theanine and amino acids in green tea separated using the Acclaim RSLC PolarAdvantage column.

Thermo SCIENTIFIC

Table of Contents

Tea: Catechins

Catechins (flavan-3-ol monomers) are abundant in teas derived from the tea plant *Camellia sinensis,* as well as in some cocoas and chocolates. The most common include catechin, epicatechin, epigallocatechin, gallocatechin, and their gallate esters. Catechins are purported to have a number of health benefits including reduction in cancer and the formation of atherosclerotic plaques.

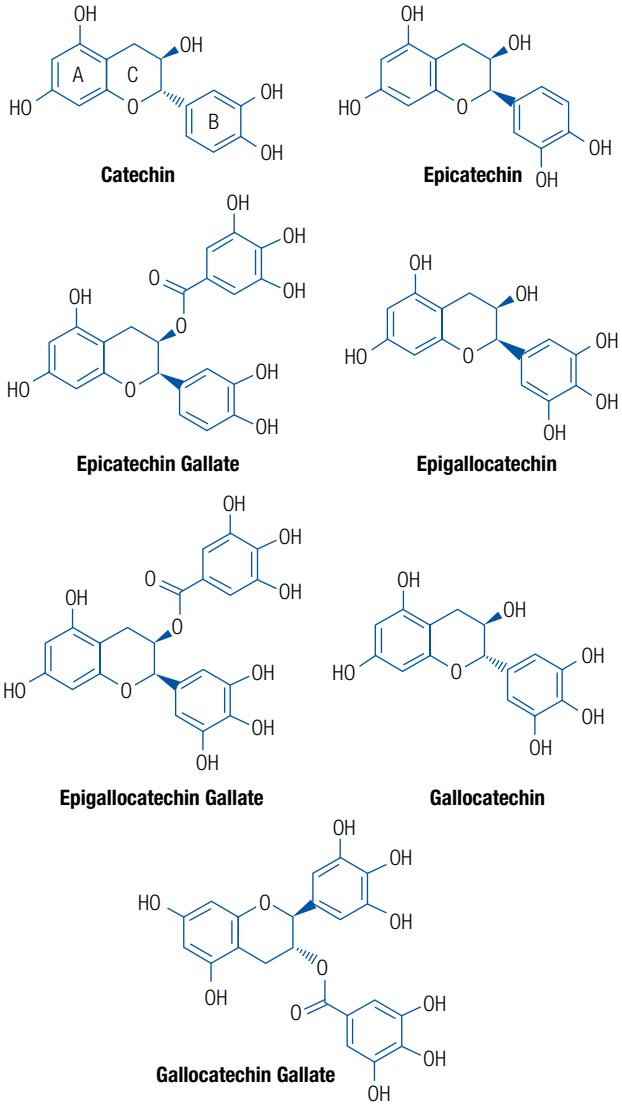


Figure 6-52. Chemical structures of catechins found in tea.

Thermo SCIENTIFIC

Tea: Catechins

Catechin concentrations were determined in a NIST control and sample prior to the analysis of commercial teas. Table 6-5 summarizes the catechin concentrations in the NIST controls and samples with a comparison to the certified values. The concentrations for all the catechins in the control were consistent with the certified NIST values.

Table 6-5. Determination of catechins in a 1:5 siluted NIST control and reference sample.

Analyte	NIST Control (mg/g)	NIST Control Certified Value (mg/g)	NIST Sample (mg/g)	NIST Sample Certified Value (mg/g)
Gallocatechin	22.8 ± 1	24 ± 1	7.84	7.60
Epigallocatechin	84.7 ± 1	88 ± 3	29.6	30.7
Catechin	9.70 ± 0.5	9.8 ± 0.4	2.46	2.60
Epicatechin	47.3 ± 1	46 ± 2	11.9	12.0
Epigallocatechin Gallate	427.3 ± 12	417 ± 16	80.8	71.1
Gallocatechin Gallate	40.9 ± 1	38 ± 3	4.46	4.60
Epicatechin Gallate	76.8 ± 2	94 ± 5	17.4	17.1
Total Catechins	709.6 ± 12.5	716.8 ± 27.4	154.5	145.7

Column: Acclaim 120, C18, 2.2 µm, analytical (2.1 × 150 mm)
Flow: 0.45 mL/min
Temperature: 25 °C
Injection Volume: 1.0 µL
Eluent: A: 0.1% TFA, 5% acetonitrile
B: 0.1% TFA in acetonitrile
Gradient: 0.0–1.2 min: 100% A, 1.2–15.5 min: 28.5% B, hold for 1.5 min at 28.5% B
Detection: Absorbance, UV 280 nm
Sample: 1:20 Dilute green tea

Peaks:	Brand A	Brand B	mg/g*
1. Gallic Acid	—	—	
2. Epigallocatechin	45.13	43.50	
3. Caffeine	—	—	
4. Catechin	3.45	3.57	
5. Epicatechin	6.14	6.08	
6. Epigallocatechin Gallate	63.98	60.56	
7. Gallocatechin Gallate	6.74	6.65	
8. Epicatechin Gallate	9.81	12.76	

*Calculated concentration

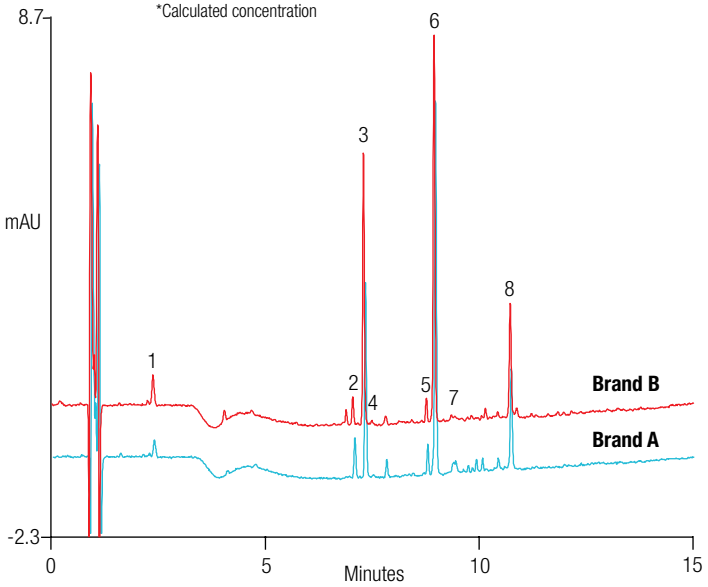


Figure 6-53. Comparison of catechins in a two different brands of green tea (diluted 1:20).

Thermo SCIENTIFIC

Tea: Catechins

Column:	Acclaim 120, C18, 2.2 µm, analytical (2.1 × 150 mm)
Flow:	0.45 mL/min
Temperature:	25 °C
Injection Volume:	1.0 µL
Eluent:	A: 0.1% TFA, 5% acetonitrile B: 0.1% TFA in acetonitrile
Gradient:	0.0–1.2 min: 100% A 1.2–15.5 min: 28.5% B Hold for 1.5 min at 28.5% B
Detection:	Absorbance, UV 280 nm
Sample:	1:20 Dilute black tea

Peaks:		
1. Gallic Acid	—	mg/g*
2. Epigallocatechin	27.77	
3. Caffeine	—	
4. Catechin	4.35	
5. Epicatechin	2.25	
6. Epigallocatechin Gallate	12.28	
7. Gallocatechin Gallate	9.20	
8. Epicatechin Gallate	7.47	

*Calculated concentration

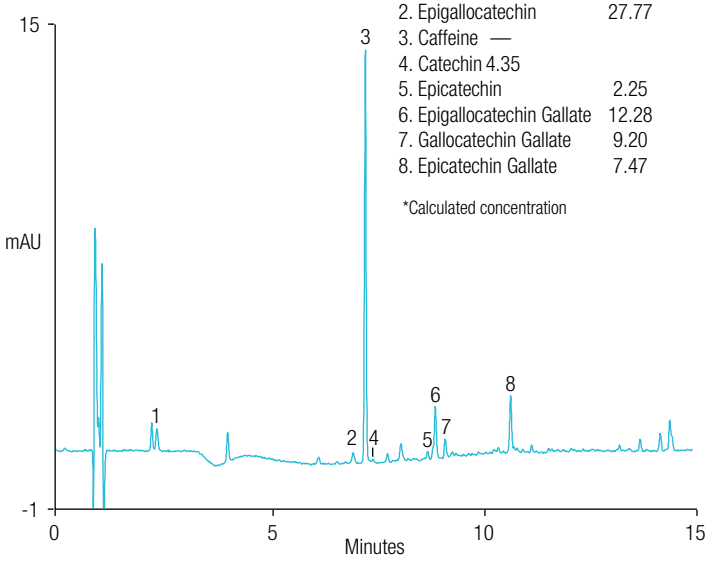


Table 6-54. Separation of catechins in a 1:20 diluted sample of black tea.

Column:	Acclaim 120, C18, 2.2 µm, analytical (2.1 × 150 mm)
Flow:	0.45 mL/min
Temp.:	25 °C
Injection Volume:	1.0 µL
Eluent:	A: 0.1% TFA, 5% acetonitrile B: 0.1% TFA in acetonitrile
Gradient:	0.0–1.2 min: 100% A 1.2–15.5 min: 28.5% B Hold for 1.5 min at 28.5% B
Detection:	Absorbance, UV 280 nm
Sample:	1:20 Dilute white tea

Peaks:		
1. Gallic Acid	—	mg/g*
2. Gallocatechin	15.77	
3. Epigallocatechin	16.51	
4. Caffeine	—	
5. Catechin	3.12	
6. Epicatechin	2.73	
7. Epigallocatechin Gallate	42.60	
8. Gallocatechin Gallate	8.83	
9. Epicatechin Gallate	8.96	

*Calculated concentration

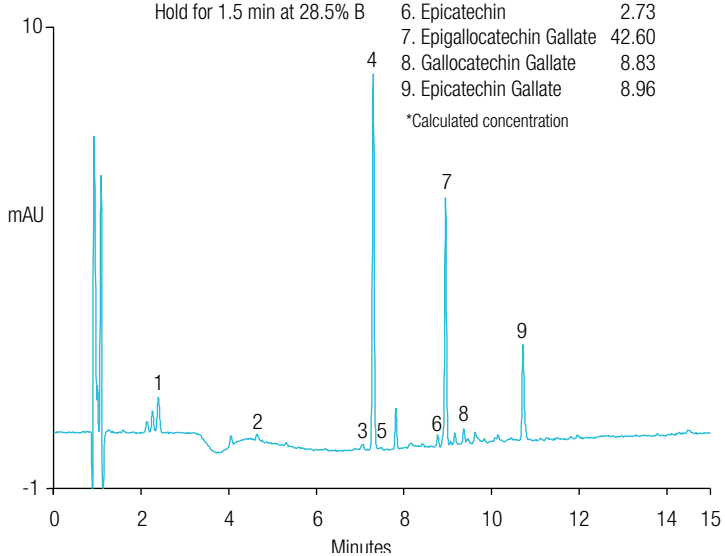
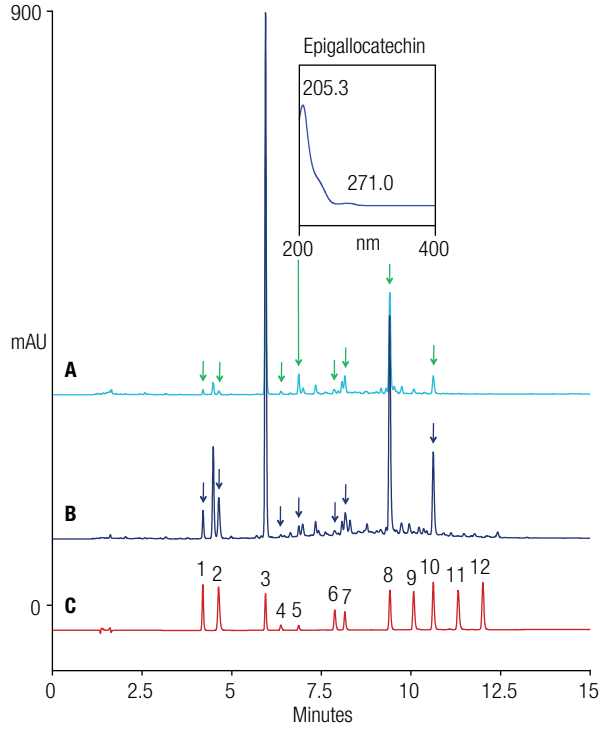


Figure 6-55. Separation of catechins in a 1:20 diluted sample of white tea.

Thermo SCIENTIFIC

Tea: Catechins



HPLC System: UltiMate 3000 RSLC
Column: Acclaim PolarAdvantage II, 3 µm, 3 × 150 mm
Flow: 0.60 mL/min
Temperature: 30 °C
Injection Volume: 5 µL
Mobile Phases: A: Acetonitrile
B: 100 mM formic acid + 20 mM ammonium formate
C: Water

Gradient Times:

	-6	0	12	15
% A:	5	5	50	50
% B:	10	10	10	10
% C:	85	85	40	40

Detection: UV at 280 nm, 5 Hz, 1 s resp. time
Samples: A. Genmai-cha green tea
B. Darjeeling black tea
C. Standards

Peaks:
1. theobromine
2. gallic acid
3. caffeine
4. gallocatechin
5. epigallocatechin
6. catechin
7. epicatechin
8. epigallocatechin gallate
9. gallocatechin gallate
10. epicatechin gallate
11. catechin gallate
12. 3,4,5-trihydroxy cinnamic acid

Figure 6-56. Comparison of catechin profiles of black and green teas using an Acclaim PolarAdvantage II column.

Did You Know?

- Tea was accidentally discovered in 2737 BC when Chinese Emperor Shen Nung found tea leaves that had blown into a pot of boiling water that produced a pleasing aroma.
- Tea was introduced to England in 1669. At that time, the drink was enjoyed only by the aristocracy because a pound of tea cost an average British laborer the equivalent of nine months in wages.

Download Application Note 275: Sensitive Determination of Catechins in Tea by HPLC

Table of Contents

Tea: Catechins

Application Brief 150 evaluates the use of an Accucore C18 HPLC column to rapidly (<6 min) determine catechins in three different types of tea. Core-shell particles improve mass transfer kinetics, and therefore separation efficiency, by restricting intra-particle diffusion to the thin, porous shell while maintaining the hydraulic permeability associated with the total particle diameter.This work demonstrates how core-shell columns can be used to increase separation efficiency with improved mass transfer kinetics without significantly increasing pressure. The Accucore C18 HPLC column enables faster separation of catechins than when using the Acclaim C18 column per the method described in AN 275.

Column:	Accucore C18, 2.6 µm, Analytical (150 × 2.1 mm)
Eluent:	A: 2.5% Acetonitrile in water B: 0.1% TFA in acetonitrile
Gradient:	0.0–1.0 min, 0% B 1.0–5.0 min, 10% B 5.0–6.0 min, 0% B
Flow Rate:	0.8 mL/min
Inj. Volume:	2.0 µL
Temperature:	42 °C
Detection:	Absorbance, UV 280 nm

Peaks:
1. Gallic Acid
2. Gallocatechin
3. Epigallocatechin
4. Catechin
5. Caffeine
6. Epicatechin
7. Epigallocatechin Gallate
8. Gallocatechin Gallate
9. Epicatechin Gallate

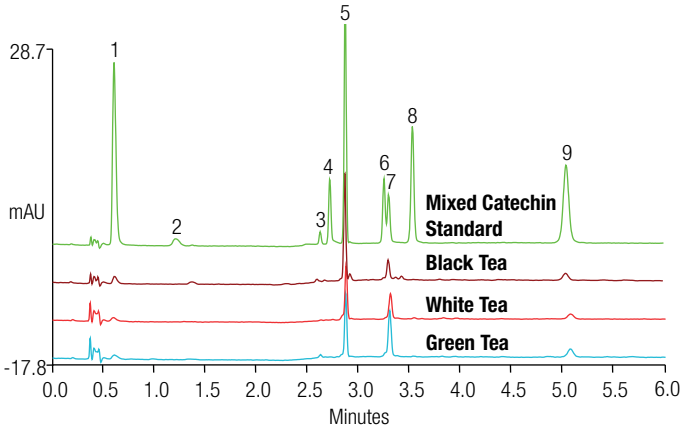


Figure 6-57. Separation of catechins in a mixed standard and three different commercially available teas using an Accucore C18 HPLC column.

Download Application Brief 150: Rapid Separation of Catechins in Tea Using Core-Shell Columns

Download Application Note 275: Sensitive Determination of Catechins in Tea by HPLC

Tea: Catechins

Catechin concentrations were determined in a NIST control and sample prior to the analysis of commercial teas. Table 6-6 summarizes the catechin concentrations in the NIST controls and samples with a comparison to the certified values. The concentrations for all the catechins in the control were consistent with the certified NIST values.

Table 6-6. Abundance of catechins in different teas. Data are in good agreement with the literature.

Compound	Green Tea (mg/g)	Black Tea (mg/g)	White Tea (mg/g)
Catechin Hydrate	3.7	3.0	8.1
Epicatechin	50.8	9.3 3	9.8
Epicatechin Gallate	65.3	40.6	95.9
Epigallocatechin	49.2	2.5	32.3
Epigallocatechin Gallate	180	31.3	211
Gallocatechin	18.8	3.2	22.0
Gallocatechin Gallate	5.9	7.0	3.0

Column: Acclaim 120, C18, 3 µm Analytical (3.0 × 150 mm, P/N 063691)
Flow Rate: 0.65 mL/min
Temperature: 35° C
Injection Volume: 20 µL
Mobile Phase: A. 20 mM Sodium Phosphate Monobasic, 3% Acetonitrile, 0.2% Tetrahydrofuran, pH 3.35
B. 20 mM Sodium Phosphate Monobasic, 50% Acetonitrile, 10% Tetrahydrofuran, pH 3.45
C. 90% Methanol
Gradient: 0–2 min, 2% B, 3% C; 30 min, 97% B, 3% C; 45 min, 97% B, 3% C; Curve 7 (concave)
Detection: UV; Channel 1, 218 nm; Channel 2, 240 nm; Channel 3, 254 nm; Channel 4, 275 nm
EC Detector Parameters: 16 Channel Array from 0 to +900 mV, relative to Pd, in 60 mV increments
Peaks:
1. Gallocatechin
2. Epigallocatechin
3. Catechin Dihydrate
4. Epicatechin
5. Epigallocatechin Gallate
6. Gallocatechin Gallate
7. Epicatechin Gallate
8. Propyl Gallate IS

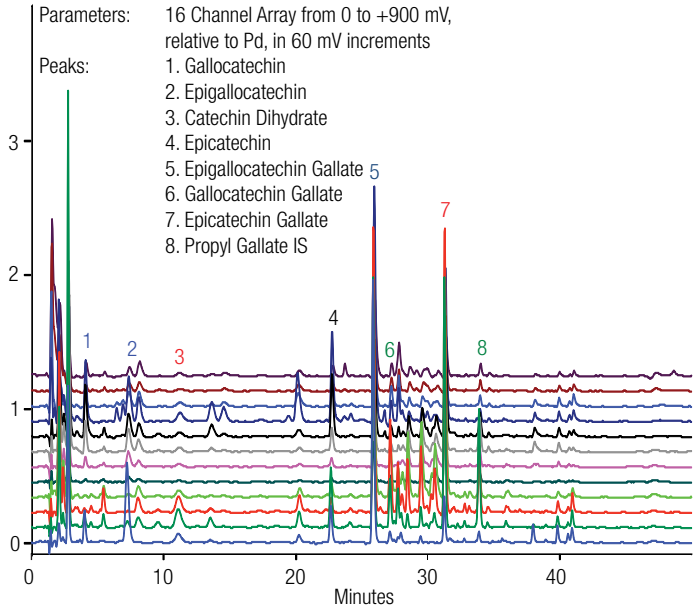


Table 6-58. Green tea EC array chromatogram presented at low sensitivity showing the highly abundant catechins.

Tea and Mango: Catechins

HPLC System:	UltiMate 3000 RSLC
Columns:	Acclaim PolarAdvantage II, 3 µm, 3 × 250 mm Guard column 5 µm, 3 × 10 mm
Flow:	0.44 mL/min
Temperature:	30 °C
Injection Volume:	10 µL
Mobile Phases:	A: Acetonitrile B: 10 mM phosphoric acid + 0.1 mM tetrasodium pyrophosphate
Gradient Times:	-13 0 43 51 % A: 5 5 60 60 % B: 95 95 40 40
Detection:	UV at 280 nm, 5 Hz, 1 s resp. time, spectra 200–500 nm
Sample:	A: Green tea B: Mango pulp

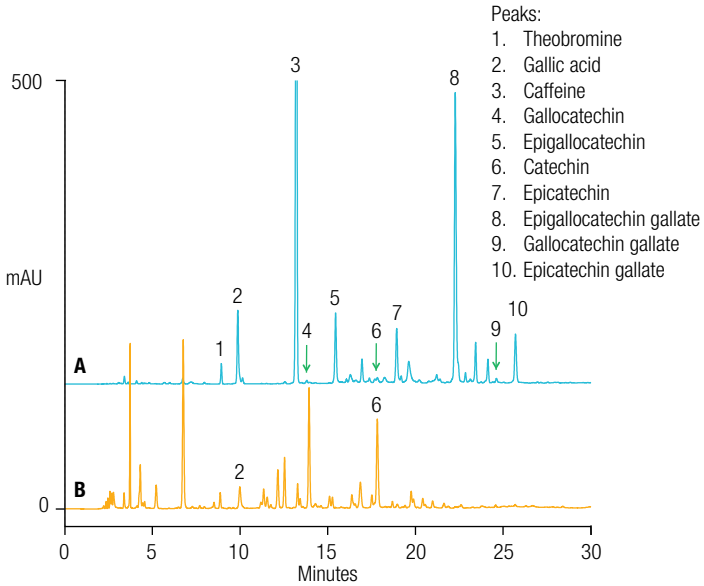


Figure 6-59. Catechins in mango and tea using an Acclaim PolarAdvantage II column.

Did You Know?

- There is only one working tea plantation in the USA and it is located on Wadmalaw Island just outside Charleston, South Carolina.
- The UK consumes 165 million cups of tea daily. The average person in the UK will consume around 80,000 cups of tea during their life.
- Apart from tourism, tea is the biggest industrial activity in India.

Tea: Inorganic Anions and Organic Acids

Table of Contents

Inorganic anions and organic acids are important constituents in tea that contribute to the quality and taste of the product.

The use of capillary ion chromatography with suppressed conductivity detection allows the simultaneous determination of several key ions in less than 30 minutes.

Did You Know?

- The Boston Tea Party ended America's liking for both the British and their tea, marked the beginning of the War of Independence, and started America's coffee-drinking tradition.
- A New York City tea importer named Thomas Sullivan invented the Tea Bag. He became annoyed at the high cost of the tin boxes he used to send tea samples to customers.

Column:	Dionex IonPac AG19, AS19, capillary (0.4 × 250 mm)
Flow Rate:	10 µL/min
Temperature:	30 °C
Injection Volume:	0.4 µL
Eluent Source:	Dionex EGC-KOH
Eluent:	15 mM KOH from 0 to 7 min, 15–60 mM from 7 to 25 min
Detection:	Suppressed conductivity, Dionex ACES 300 suppressor
Sample:	English breakfast tea
Peaks:	1. Chloride 2. Nitrate 3. Sulfate 4. Malate 5. Phosphate 6. Citrate

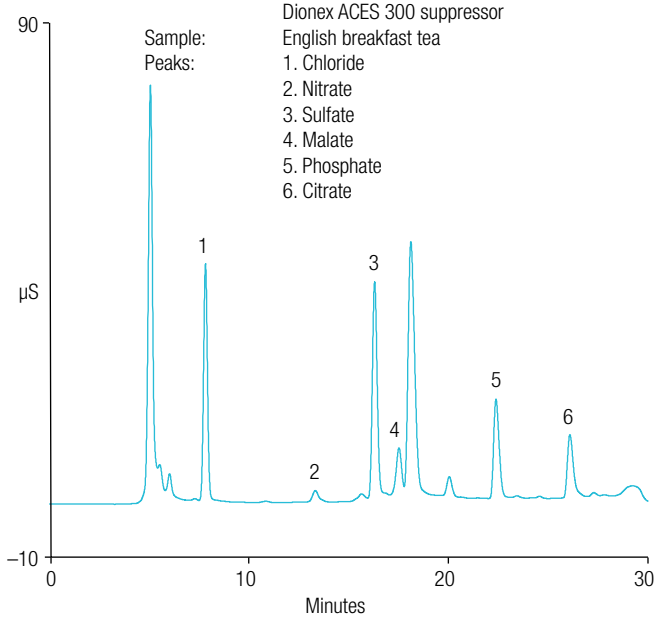


Figure 6-60. Determination of inorganic anions and organic acids in tea by capillary ion chromatography

Thermo SCIENTIFIC

Table of Contents

Profiling Beverages

Red, white and blush wines

Wine

Wine is an alcoholic beverage made from fermented grapes or other fruits. Wine has a rich history dating back thousands of years, with the earliest production occurring c. 6000 BC in Georgia. Different varieties of grapes and strains of yeasts produce different styles of wine. Varietals result from the very complex interactions between the development of the fruit and reactions involved in fermentation, as well as effects of growing region, soil, climate and human intervention in the overall process. Important biochemicals can be analyzed using HPLC- and IC-based approaches.

Thermo SCIENTIFIC

Wine: Anions and Organic Acids

The flavors imparted by wine are in part due to its organic acid composition. Tartaric, citric, and malic acids are the three major organic acids found naturally in wines. The maturation of a wine can be followed by changes in organic acid composition. For example, as many red wines age, the concentration of free tartaric acid decreases as it precipitates by binding with other components of the wine. Organic acids also contribute to the overall acidity and tartness of a wine and can contribute flavors that are either pleasing or undesirable. For example, malic acid can impart a green apple flavor, whereas excessive acetic acid will impart an unwanted vinegar flavor. Malolactic fermentation is a winemaking technique popular for the production of some chardonnays. In this process, the malic acid is converted to lactic acid by bacteria, either naturally or by the specific introduction of the bacteria, to produce a wine with a lower acidity and different taste.

Application Note 273 describes the use of ion chromatography (IC) with suppressed conductivity detection to separate a large variety of organic acids and detect them with high sensitivity, along with inorganic anions, in different wine samples.

Table 6-7. Gradient for Figure 6-58.

Time	%A	%B	%C	%D
–15.0	80	0	0	20
–10.0	80	0	0	20
–9.5	0	97	3	0
0.0	0	97	3	0
3.5	0	97	3	0
3.6	0	92	8	0
9.0	0	92	8	0
28.0	0	0	100 (Curve 7)	0
35.0	0	0	100	0

Column: Thermo Scientific™ OmniPac™ PAX-100 Analytical, 4 × 250 mm
OmniPac PAX-100 Guard, 4 × 50 mm
Trap Column: Dionex IonPac ATC-HC, 9 × 75 mm
Temperature: 30 °C
Flow: 1.0 mL/min
Injection Volume: 25 µL
Eluent: A: DI water
B: 12% Methanol/16% ethanol in DI water
C: 0.1 M Sodium hydroxide
D: 1 M Sodium hydroxide

Gradient: See Table 6-5
Detection: Suppressed conductivity
Suppressor: Dionex AMMS 300 suppressor, 4 mm
Sample: Mixture of standards
Regenerant: 20 mN H_2SO_4

Sample: Wine Samples
A. Red Wine 1
B. Red Wine 2
C. White Wine 1
D. White Wine 2

Peaks:	A	B	C	D
2. Acetate	4.66	5.47	5.02	6.96 mg/L
3. Lactate	12.8	14.4	2.98	8.43
5. Shikimate	0.11	0.12	0.05	0.06
6. Chloride	1.76	0.37	0.31	1.44
9. Nitrate	0.11	0.07	0.05	0.06
10. Succinate	7.20	8.02	3.46	6.63
11. Malate	0.51	2.37	14.3	3.64
12. Tartarate	22.66	16.6	10.9	—
13. Sulfate	2.68	3.89	2.43	1.80
14. Oxalate	0.04	0.04	0.03	0.05
15. Phosphate	8.10	5.47	3.98	1.33
16. Citrate	0.14	0.55	2.27	14.6

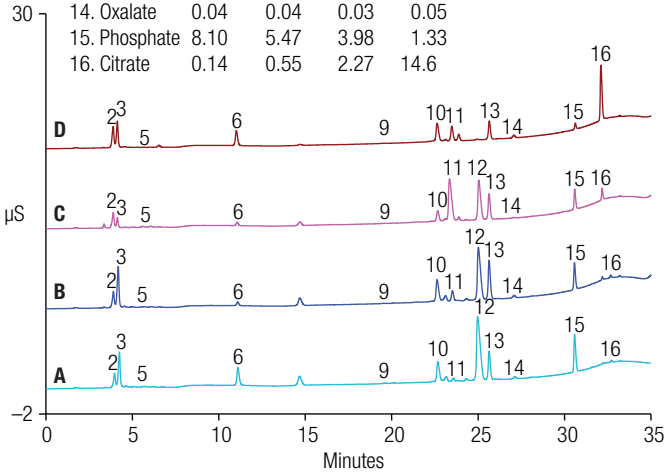


Figure 6-61. Chromatograms of the four wine samples.

Download Application Note 273: Higher Resolution Separation of Organic Acids and Common Inorganic Anions in Wine

Wine: Anions and Organic Acids

Table 6-8. Amount of anions and organic acids in wine samples (100 × dilution).

Analyte	Red Wine 1		Red Wine 2		White Wine 1		White Wine 2	
	Average (mg/L)	RSD (n=3)	Average (mg/L)	RSD (n=3)	Average (mg/L)	RSD (n=3)	Average (mg/L)	RSD (n=3)
Fluoride	—	—	—	—	—	—	—	—
Acetate	4.66	0.91	5.47	0.52	5.02	1.51	6.96	0.60
Lactate	12.8	1.42	14.4	0.87	2.98	2.27	8.43	0.65
Formate	–	–	—	—	—	—	—	—
Shikimate	0.11	2.242	0.12	3.53	0.05	4.72	0.06	9.91
Chloride	1.76	1.20	0.37	0.45	0.31	2.05	1.44	0.80
Nitrite	—	—	—	—	—	—	—	—
Bromide	—	—	—	—	—	—	—	—
Nitrate	0.11	0.92	0.07	0.70	0.05	2.31	0.06	10.48
Succinate	7.20	1.07	8.02	0.35	3.46	1.41	6.63	1.22
Malate	0.51	1.41	2.37	0.57	14.3	1.35	3.64	1.37
Tartarate	22.6	0.96	16.6	0.34	10.9	1.47	—	—
Sulfate	2.68	1.09	3.89	0.45	2.43	1.80	1.80	1.34
Oxalate	0.04	0.77	0.04	1.79	0.03	4.77	0.05	1.98
Phosphate	8.10	0.95	5.47	0.50	3.98	1.68	1.33	2.16
Citrate	0.14	1.04	0.55	0.76	2.27	1.59	14.6	1.43

Thermo SCIENTIFIC

Wine: Catechins and Phenolic Acids

Dietary polyphenols comprise a wide range of aromatic compounds that are responsible for numerous organoleptic characteristics of plant-derived food and beverages. In addition to color and taste properties, polyphenols are reported to have antioxidant characteristics, making them responsible for the healthy features of fruit, vegetables, and plant-derived beverages.

The polyphenols that are present in foods can be divided into two main groups: non-flavonoids and flavonoids. Non-flavonoids are mostly monocyclic acids and can be further divided into two main sub-classes: phenolic acids and stilbenes (e.g. resveratrol). Phenolic acids are subdivided into benzoic acids and hydroxycinnamic acids.

Flavonoids share a common nucleus consisting of two phenolic rings and an oxygenated heterocycle. They form a diverse range of compounds include anthocyanins, flavonols, flavanols, flavones, and chalcones. The catechin group of flavanols are major components in wine and are reported to have antioxidant, antimicrobial, antimutagenic and anticarcinogenic activities.

Application Note 20583 demonstrates the use of SPE along with a simple and rapid HPLC-UV method for the analysis of nine catechins and phenolic acids in red wine.

Column:	Accucore PFP 2.6 µm, 100 mm × 2.1 mm (PN 17426-102130)
Flow:	0.4 mL/min
Column Temp.:	30 °C
Autosampler Temp.:	Ambient
Injection Volume:	1 µL
Mobile Phase:	A: Water + 0.1% formic acid
	B: acetonitrile + 0.1% formic acid
Gradient:	Time (min) % B
	0 2
	0.1 2
	7.1 65
	7.2 95
	7.9 95
	8.0 2
	10.0 2
Detection:	UV at 280 nm
Run Time:	10 min
Syringe Fush:	Mobile phase

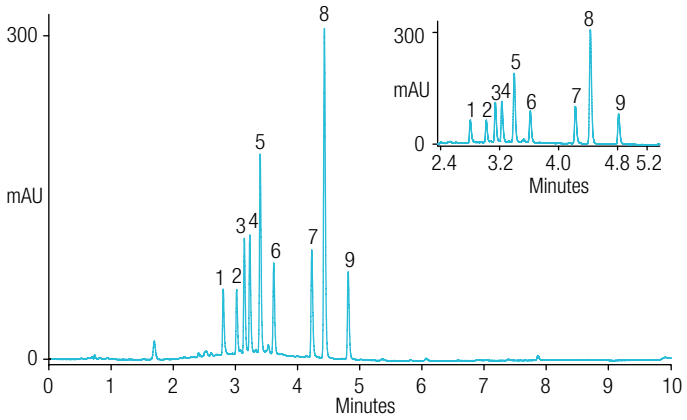


Figure 6-62. Chromatogram for standard mixture 1, containing nine polyphenol standards prepared in a red wine matrix and extracted by SPE. Order of elution: 1. catechin; 2. epicatechin; 3. syringic acid; 4. gallocatechin gallate; 5. hydroxybenzaldehyde; 6. p-vanillin; 7. myricetin; 8. resveratrol; 9. quercetin.

Download Application Note 20583: Determination of Catechins and Phenolic Acids in Red Wine by Solid Phase Extraction and HPLC

Wine: Inorganic and Organic Acids

Conditions for Figures 6-58a, 6-58b and 6-58c

Columns: Dionex IonPac AS11-HC-4 µm Guard, 2 × 50 mm (P/N 078036)
Dionex IonPac AS11-HC-4 µm Analytical, 2 × 250 mm (P/N 078035)
Flow: 0.4 mL/min
Injection Volume: 2.5 µL
Eluent Source: Dionex EGC 500 KOH Eluent Generator Cartridge with Dionex CR-ATC 500 Continuously Regenerated Anion Trap Column
Eluent: A: DI Water
B: CH_3OH

Time (min)	KOH (mM)	Time (min)	B (%)
-2.000	1	-2.000	8
0.000	1	0.000	8
10.070	1	19.000	8
10.071	1	20.000	11
24.000	15	30.000	11
24.010	15	31.000	8
35.000	27	33.000	8
40.000	60	33.010	0
44.000	60	44.000	0
44.010	1	44.010	8
45.000	1	45.000	8

Detection: Suppressed Conductivity, Dionex ASRS 300 Anion Self-Regenerating Suppressor (2 mm),* 82 mA, external water mode
System Backpressure: ~3900 psi (1 mM KOH/8% CH_3OH), ~4800 psi (60 mM KOH/11% CH_3OH)
Background Conductance: ~0.16–0.7- µS
Noise: ~0.6–0.9 nS/min, peak-to-peak
Run Time: 47 min

* Equivalent or improved results can be achieved on the Thermo Scientific™ Dionex™ AERS 500 Anion Electrolytically Regenerated Suppressor.

Peaks:		A		B
	1. Quinate	4.31	mg/L	4.31
	2. Fluoride	0.508		0.508
	3. Lactate	79.9		79.9
	4. Acetate	21.3		21.3
	5. Glycolate	2.05		2.05
	6. Galacturonate	59.7		120
	7. Chloride	1.41		1.41
	8. Nitrate	0.578		0.578
	9. Succinate	33.2		33.2
	10. Malate	11.2		43.3
	11. Carbonate	—		—
	12. Tartrate	99.6		193
	13. Maleate	5.31		5.31
	14. Sulfate	20.1		20.1
	15. Oxalate	0.145		0.145
	16. Phosphate	42.6		42.6
	17. Citrate	4.61		8.76
	18. Isocitrate	1.96		1.96
	19. *cis*-Aconitate	0.450		0.450
	20. *trans*-Aconitate	0.0626		0.0626

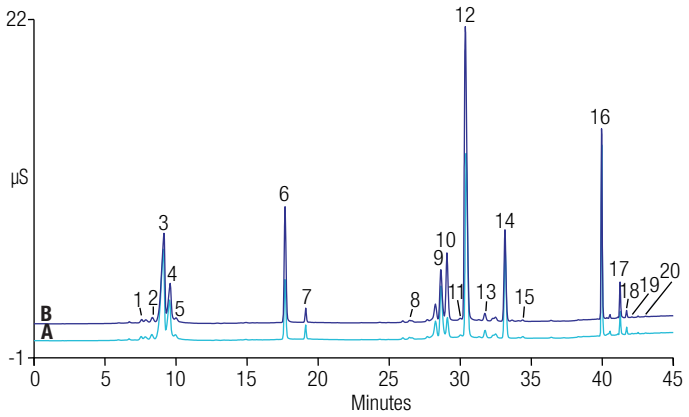


Figure 6-63. (A) Merlot wine and (B) spiked Merlot wine analyzed on the Dionex IonPac AS11-HC-4 µm column.

Wine: Inorganic and Organic Acids

		A		B				
Peaks:	1. Quinate	6.01	mg/L	6.01	13. Carbonate	—	—
	2. Fluoride	1.59		1.59	14. Tartrate	83.7	163
	3. Lactate	47.0		47.0	15. Maleate	12.6	12.6
	4. Acetate	14.0		14.0	16. Sulfate	18.3	18.3
	5. Glycolate	1.97		1.97	17. Fumarate	0.0390	0.0390
	6. Formate	0.149		0.149	18. Oxalate	0.402	0.402
	7. Pyruvate	0.908		0.908	19. Phosphate	25.5	25.5
	8. Galacturonate	20.7		42.0	20. Citrate	20.5	41.0
	9. Chloride	1.53		1.53	21. Isocitrate	2.38	2.38
	10. Nitrate	0.555		0.555	22. *cis*-Aconitate	0.117	0.117
	11. Succinate	14.7		14.7	23. *trans*-Aconitate	0.0496	0.0496
	12. Malate	117		232			

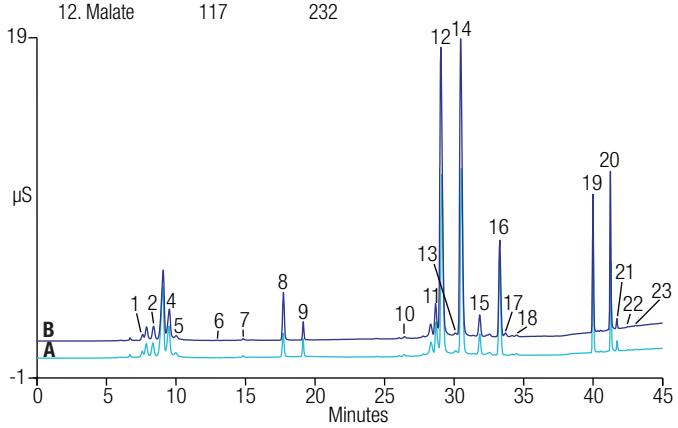


Figure 6-64. A) White Zinfandel wine and (B) spiked White Zinfandel wine analyzed on the Dionex IonPac AS11-HC-4 µm column.

		A		B			
Peaks:	1. Quinate	3.01	mg/L	3.01	12. Carbonate	—	—
	2. Fluoride	1.12		1.12	13. Tartrate	108	212
	3. Lactate	26.1		26.1	14. Maleate	12.8	12.8
	4. Acetate	8.08		8.08	15. Sulfate	16.2	16.2
	5. Glycolate	1.39		1.39	16. Fumarate	0.134	2.20
	6. Pyruvate	0.907		0.907	17. Oxalate	0.335	0.335
	7. Galacturonate	31.9		63.1	18. Phosphate	27.5	27.5
	8. Chloride	2.25		2.25	19. Citrate	29.4	59.7
	9. Nitrate	0.850		0.850	20. Isocitrate	2.31	2.31
	10. Succinate	13.6		13.6	21. *cis*-Aconitate	0.187	0.187
	11. Malate	175		338	22. *trans*-Aconitate	0.0563	0.0563

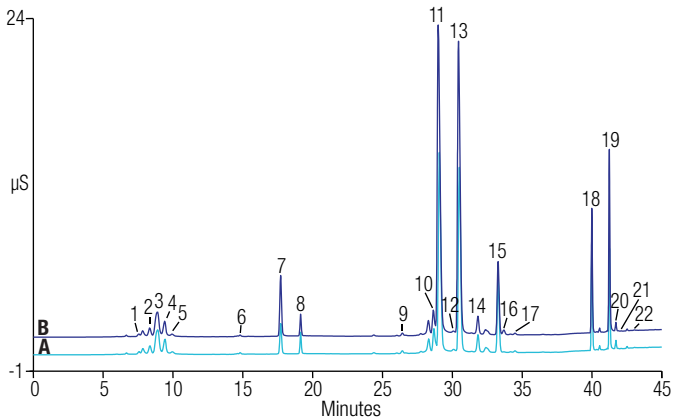


Figure 6-65. (A) Chardonnay wine and (B) spiked Chardonnay wine analyzed on the Dionex IonPac AS11-HC-4 µm column.

Thermo SCIENTIFIC

Wine: Polyphenols

Gradient HPLC, with our unique Spectro-Electro Array detection, is both selective and sensitive and can be used to simultaneously measure hundreds of known and unknown secondary metabolites in a sample, without the need for solid phase extraction.

Did You Know?

- California produces over 17 million gallons of wine each year.
- The Mesopotamians were credited with producing the first wines in 6000 B.C.
- In France (and many other European countries) the government regulates a designated growing area. The name of the growing area is called an appellation.

Table 6-9. Some of the more abundant analytes measured in different wine samples and in good agreement with literature. Wine 1: Cabernet Sauvignon, Argentina; Wine 2: Cabernet Sauvignon, South Africa; Wine 3: Cabernet Sauvignon, US; Wine 4: Cabernet Sauvignon, Chile; Wine 5: Hearty Burgundy, US.

Compound	Wine #1 mg/L	Wine #2 mg/L	Wine #3 mg/L	Wine #4 mg/L	Wine #5 mg/L
Apigenin	16	17.5	9.5	13	41
Caffeic acid	8	13	5	17	3
Catechin	37	26	26.5	24	22
Ellagic acid	52	133	84	94	100
Epicatechin	19	15	16.5	11	4
Ferulic acid	1	1	2	3	2
Gallic acid	57	33.5	37	35	29.5
Isorhamnetin	6	5.5	2.5	6.5	2
Kaempferol	0.5	0.5	0.5	1	1
Myricetin	11	11	5	8	1.5
p-coumaric acid	8.5	16	2.5	14.5	3.5
Quercetin	13.5	15.5	3	14	4
Resveratrol – *cis*	1	1.5	0.5	2	0.5
Resveratrol – *trans*	2.5	2	1	2.5	1.5
Sinapic acid	2	2	2	2	2
Syringic acid	19	9.5	9	12	7
Vanillic acid	6.5	4.5	2.5	8	4

Thermo SCIENTIFIC

Wine: Polyphenols

Pump:	LPG-3400 BM with SR-3000 Solvent Rack
Column:	Acclaim 120, C18, 3 × 150 mm, 3 µm
Flow:	0.65 mL/min
Injection Volume:	10 or 20 µL
Mobile Phases:	A. 20 mM monobasic sodium phosphate, 3% acetonitrile, 0.2% tetrahydrofuran, pH 3.35 B. 20 mM monobasic sodium phosphate, 50% acetonitrile, 10% tetrahydrofuran, pH 3.45 C. 90% methanol
Gradient:	0-2 min: 2% B /3% C. 30 min: 97% B/3% C, 45 min 97% B/3% C. Curve 7 (concave).
Autosampler:	WPS-3000TBSL
UV Detector:	DAD-3000RS Diode-Array Detector Channel 1: 218 nm, channel 2: 240 nm, channel 3: 254 nm, channel 4: 275 nm
EC Detector:	CoulArray Detector with Thermal Organizer
EC Parameters:	16 channel array from 0 to +900 mV in +60 mV increments

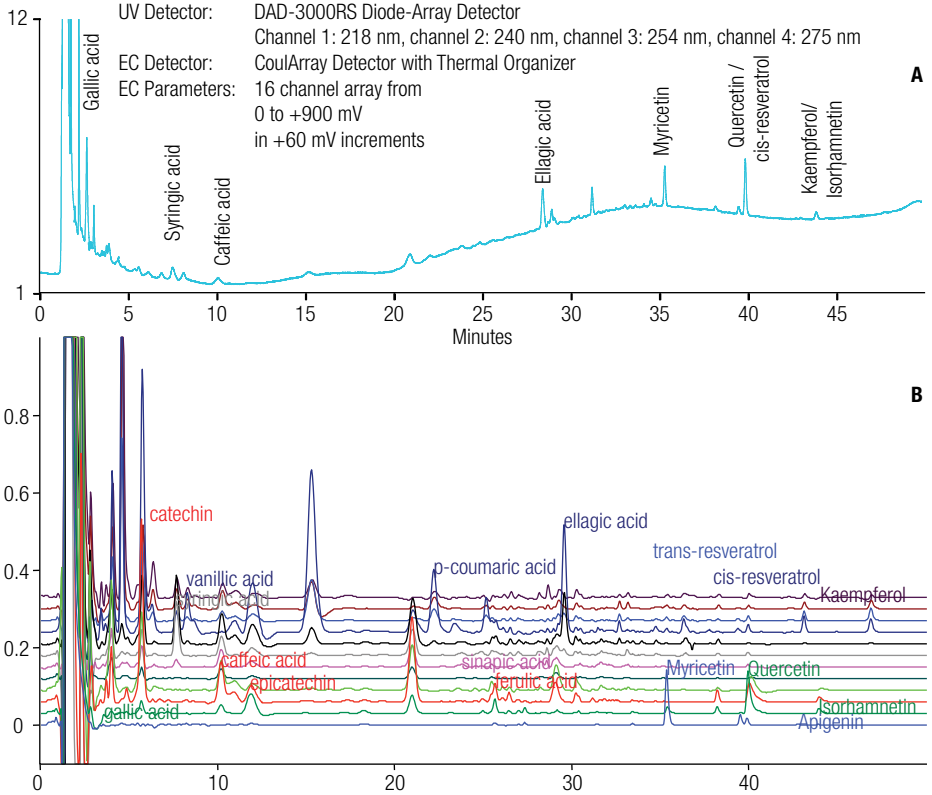


Figure 6-66. A) Wine Sample 1 (Cabernet Sauvignon, Argentina) analyzed by UV at 254 nm. B) Same sample analyzed using EC array detection (presented at low sensitivity). Note that compounds that co-elute by UV detection are fully resolved using EC array detection (e.g., quercetin/*cis*-resveratrol; kaempferol/isorhamnetin).

Table of Contents

Wine: Resveratrol

Resveratrol (3,5,4'-trihydroxy-*trans*-stilbene), a stilbenoid, is associated with the health benefits of drinking red wine.

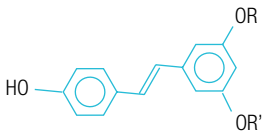
Did You Know?

- There are 24,000 names for varieties of wine grapes, corresponding to between 5,000 and 10,000 actual varieties. However, only about 150 are commercially important.
- There is about 90 pounds per square inch pressure in a bottle of Champagne, approximately three times the pressure in your automobile tires..

LC System:	UltiMate 3000 RSLC				
Column:	Acclaim RSLC PA2, 3 µm, 3.0 × 250 mm				
Flow:	0.60 mL/min				
Temperature:	25 °C				
Injection Volume:	2 µL				
Mobile Phases:	A. Methanol				
	B. 0.02% H_3PO_4 (v/v)				
Gradient Time (min):	–10	0	2	20	27
%A	45	45	45	95	95
%B	55	55	55	5	5
Detection:	UV at 310 nm				
	Spectral confirmation, 200–450 nm				

Peaks:

	R	R'
1. Polydatin	H	Glucose
2. Resveratrol	H	H
3. Pterostilbene	CH_3	CH_3



Sample Preparation:
1. 5.0 mL Zinfandel red wine
2. Fortify to 2 µg/mL resveratrol
3. Extract with 2 × 1 mL ethyl acetate
4. Weight of combined extracts approx. 1.5 g

Figure 6-67. Separation of resveratrol in red wine on the Acclaim RSLC PolarAdvantage II (PA2) column.

Download Application Note 1064: Product Authentication and Adulteration Determination Using a Novel Spectro-Electro Array Platform

Download Application Brief 164: Measurement of Resveratrol, Kaempferol, Quercetin and Isorhamnetin in Human Plasma

References

Technical Collateral and Peer Reviewed Journals

Here you'll find a multitude of references using our HPLC, ion chromatography and sample preparation solutions.

Thermo SCIENTIFIC

Table of Contents

References

HPLC and UHPLC References

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Carbohydrates

Title	Authors	Publication	Publication Date
Carbohydrate and oligosaccharide analysis with a universal HPLC detector.	Asa, D.	*American Laboratory 38,* 16.	2006
Determination of levoglucosan in atmospheric aerosols using high performance liquid chromatography with aerosol charge detection.	Dixon, R. W.; Baltzell, G.	*J. Chromatogr., A. 1109 (2),* 214–221	2006 Mar 24
Composition of structural carbohydrates in biomass: Precision of a liquid chromatography method using a neutral detergent extraction and a charged aerosol detector.	Godin, B.; Agneessens, R.; Gerin, P. A.; Delcarte, J.	*Talanta 85 (4),* 2014–2026	2011 Sep 30
Selectivity issues in targeted metabolomics: Separation of phosphorylated carbohydrate isomers by mixed-mode hydrophilic interaction/weak anion exchange chromatography.	Hinterwirth, H.; Lämmerhofer, M.; Preinerstorfer, B.; Gargano, A.; Reischl, R.; Bicker, W.; Trapp, O.; Brecker, L.; Lindner, W.	*J. Sep. Sci. 33 (21),* 3273–3282	2010 Nov
Investigation of polar organic solvents compatible with Corona charged aerosol detection and their use for the determination of sugars by hydrophilic interaction liquid chromatography.	Hutchinson, J. P.; Remenyi, T.; Nesterenko, P.; Farrell, W.; Groeber, E.; Szucs, R.; Dicinoski, G.; Haddad, P. R.	*Anal. Chim. Acta. 750,* 199–206	2012 Oct 31
Characterization of an endoglucanase belonging to a new subfamily of glycoside hydrolase family 45 of the basidiomycete Phanerochaete chrysosporium.	Igarashi, K.; Ishida, T.; Hori, C.; Samejima, M.	*Appl. Environ. Microbiol. 74 (18),* 5628–5634	2008 Sep
Direct detection method of oligosaccharides by high-performance liquid chromatography with charged aerosol detection.	Inagaki, S.; Min, J. Z.; Toyo'oka, T.	*Biomed. Chromatogr. 21 (4),* 338–342	2007 Apr
Differential selectivity of the Escherichia coli cell membrane shifts the equilibrium for the enzyme-catalyzed isomerization of galactose to tagatose.	Kim, J. H.; Lim, B. C.; Yeom, S. J.; Kim, Y. S.; Kim, H. J.; Lee, J. K.; Lee, S. H.; Kim, S. W.; Oh, D. K.	*Appl. Environ. Microbiol. 74 (8),* 2307–2313	2008 Apr
Elution strategies for reversed-phase high-performance liquid chromatography analysis of sucrose alkanoate regioisomers with charged aerosol detection.	Lie, A.; Pedersen, L. H.	*J. Chromatogr., A. 1311,* 127–133	2013 Oct 11
Design of experiments and multivariate analysis for evaluation of reversed-phase high-performance liquid chromatography with charged aerosol detection of sucrose caprate regioisomers	Lie, A.; Wimmer, R.; Pedersen, L. H.	*J. Chromatogr., A. 1281,* 67–72	2013 Mar 15
Solvent effects on the retention of oligosaccharides in porous graphitic carbon liquid chromatography	Melmer, M.; Stangler, T.; Premstaller, A.; Lindner, W.	*J. Chromatogr., A 1217 (39)* 6092–6096	2010 Sep 24
Practical preparation of lacto-N-biose I, a candidate for the bifidus factor in human milk	Nishimoto, M.; Kitaoka, M.	*Biosci., Biotechnol., Biochem. 71 (8),* 2101–2104	2007 Aug

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Carbohydrates

Title	Authors	Publication	Publication Date
Cellotriose and cellotetraose as inducers of the genes encoding cellobiohydrolases in the basidiomycete Phanerochaete chrysosporium	Suzuki, H.; Igarashi, K.; Samejima, M.	*Appl. Environ. Microbiol. 76 (18),* 6164–6170	2010 Sep
1,2-alpha-l-Fucosynthase: A glycosynthase derived from an inverting alpha-glycosidase with an unusual reaction mechanism	Wada, J.; Honda, Y.; Nagae, M.; Kato, R.; Wakatsuki, S.; Katayama, T.; Taniguchi, H.; Kumagai, H.; Kitaoka, M.; Yamamoto, K.	*FEBS Lett. 582 (27),* 3739–3743	2008 Nov 12
Efficient separation of oxidized cello-oligosaccharides generated by cellulose degrading lytic polysaccharide monooxygenases	Westereng, B.; Agger, J. W.; Horn, S. J.; Vaaje-Kolstad, G.; Aachmann, F. L.; Stenstrøm, Y. H.; Eijsink, V. G.	*J. Chromatogr., A. 1271 (1),* 144–152	2013 Jan 4
Distribution of in vitro fermentation ability of lacto-*N*-Biose I, a major building block of human milk oligosaccharides, in bifidobacterial strains	Xiao, J. Z.; Takahashi, S.; Nishimoto, M.; Odamaki, T.; Yaeshima, T.; Iwatsuki, K.; Kitaoka, M.	*Appl. Environ. Microbiol. 76 (1),* 54–59	2010 Jan

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Characterization of phenolic compounds in strawberry (Fragaria x ananassa) fruits by different HPLC detectors and contribution of individual compounds to total antioxidant capacity	Aaby, K.; Ekeberg, D.; Skrede, G.	*J. Agric. Food Chem. 55 (11),* 4395–4406	2007 May 30
Analysis of flavonoids and other phenolic compounds using high-performance liquid chromatography with coulometric array detection: relationship to antioxidant activity	Aaby, K.; Hvattum, E.; Skrede, G.	*J. Agric. Food Chem. 52 (15),* 4595–4603	2004 Jul 28
Aqueous extract of Astragali Radix induces human natriuresis through enhancement of renal response to atrial natriuretic peptide	Ai, P.; Yong, G.; Dingkun, G.; Qiuyu, Z.; Kaiyuan, Z.; Shanyan, L.	*J. Ethnopharmacol. 116 (13),* 413–421	2008 Mar 28
Antioxidant, α-amylase inhibitory and oxidative DNA damage protective property of *Boerhaavia diffusa* (Linn.) root	Akhter, F.; Hashim, A.; Khan, M. S.; Ahmad, S.; Iqbal, D.; Srivastava, A. K.; Siddiqui, M. H.	*S. Afr. J. Bot. 88,* 265–272	2013 Sep
Antioxidant activity and metabolite profile of quercetin in vitamin-E-depleted rats.	Ameho, C. K.; Chen, C. Y. O.; Smith, D.; Sánchez-Moreno, C.; Milbury, P. E.; Blumberg, J. B.	*J. Nutr. Biochem. 19 (7),* p.467–474	2008 Jul
Evaluation of tolerable levels of dietary quercetin for exerting its antioxidative effect in high cholesterol-fed rats	Azuma, K.; Ippoushi, K.; Terao, J.	*Food Chem. Toxicol. 48 (4),* 1117–1122	2010 Apr
Recent methodology in ginseng analysis	Baek, S.; Bae, O.; Park, J.	*J. Ginseng Res. 36 (2),* 119–134	2012 Apr
Sensitive determination of saponins in radix et rhizoma notoginseng by charged aerosol detector coupled with HPLC	Bai, C.; Han, S.; Chai, X.; Jiang, Y.; Li, P.; Tu, P.	*J. Liq. Chromatogr. Relat. Technol. 32 (2),* 242–260	2010 Aug 27
Comprehensive analysis of polyphenols in 55 extra virgin olive oils by HPLC-ECD and their correlation with antioxidant activities	Bayram, B.; Esatbeyoglu, T.; Schulze, N.; Ozcelik, B.; Frank, J.; Rimbach, G.	*Plant Foods Hum. Nutr. (N. Y., NY, U.S.) 67 (4),* 326–336	2012 Dec
Hydrogen sulfide mediates the vasoactivity of garlic	Benavides, G. A.; Squadrito, G. L.; Mills, R. W.; Patel, H. D.; Isbell, T. S.; Patel, R. P.; Darley-Usmar, V. M.; Doeller, J. E.; Kraus, D. W.	*Proc.Natl. Acad. Sci. U.S.A. 104 (46),* 17977–17982	2007 Nov
Analysis of selected stilbenes in Polygonum cuspidatum by HPLC coupled with CoulArray detection	Benová, B.; Adam, M.; Onderková, K.; Královský, J.; Krajícek, M.	*J. Sep. Sci. 31 (13),* 2404–2409	2008 Jul
Rapid and complete extraction of phenols from olive oil and determination by means of a coulometric electrode array system	Brenes, M.; García, A.; García, P.; Garrido, A.	*J. Agric. Food Chem. 48 (11),* 5178–5183	2000 Nov
The real nature of the indole alkaloids in *Cortinarius infractus:* Evaluation of artifact formation through solvent extraction method development	Brondz, I.; Ekeberg, D.; Høiland, K.; Bell, D.; Annino, A.	*J. Chromatogr., A 1148 (1),* 1–7	2007 Apr 27

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Chemotaxonomic differentiation between Cortinarius infractus and Cortinarius subtortus by supercritical fluid chromatography connected to a multi-detection system	Brondz, I.; Høiland, K.	*Trends Chromatogr. 4,* 79–87	2008
Carotenoid bioavailability is higher from salads ingested with full-fat than with fat-reduced salad dressings as measured with electrochemical detection	Brown, M. J.; Ferruzzi, M. G.; Nguyen, M. L.; Cooper, D. A.; Eldridge, A. L.; Schwartz, S. J.; White, W. S.	*Am. J. Clin. Nutr.* 80 (2), 396–403	2004 Aug
Naringenin from cooked tomato paste is bioavailable in men	Bugianesi, R.; Catasta, G.; Spigno, P.; D'Uva, A.; Maiani, G.	*J. Nutr.* 132 (11), 3349–3352	2002 Nov
"Dilute-and-shoot" triple parallel mass spectrometry method for analysis of vitamin D and triacylglycerols in dietary supplements	Byrdwell, W. C.	*Anal. Bioanal. Chem. 401 (10),* 3317–3334	2011 Dec
Human skeletal muscle ascorbate is highly responsive to changes in vitamin C intake and plasma concentrations	Carr, A. C.; Bozonet, S. M.; Pullar, J. M.; Simcock, J. W.; Vissers, M. C.	Am. J. Clin. Nutr. 97 (4), 800–807	2013 Apr
Utilization of RP-HPLC fingerprinting analysis for the identification of diterpene glycosides from *Stevia rebaudiana*	Chaturvedula, V.; Prakash, I.	*Int. J. Res. Phytochem. Pharmacol. 1 (2),* 88–92	2011 Jun 9
Acid and alkaline hydrolysis studies of stevioside and rebaudioside A	Chaturvedula, V.; Prakash, I.	*J. Appl. Pharm. Sci. 1 (8),* 104–108	2011 Oct
Spectral analysis and chemical studies of the sweet constituent, rebaudioside A	Chaturvedula, V.; Prakash, I.	*Eur. J. Med. Plants 2 (1),* 57–65	2012 Feb
Flavonoids from almond skins are bioavailable and act synergistically with vitamins C and E to enhance hamster and human LDL resistance to oxidation	Chen, C.; Milbury, P. E.; Lapsley, K.; Blumberg, J. B.	*J. Nutr. 135 (6),* 1366–1373	2005 Jun 1
Photostability of rebaudioside A and stevioside in beverages	Clos, J. F.; Dubois, G. E.; Prakash, I.	*J. Agric. Food Chem. 56 (18),* 8507–8513	2008 Sep 24
CoulArray electrochemical evaluation of tocopherol and tocotrienol isomers in barley, oat and spelt grains	Colombo, M. L.; Marangon, K.; Bugatti, C.	*Nat. Prod. Commun. 4 (2),* 251–254	2009 Feb
Composition and stability of phytochemicals in five varieties of black soybeans (Glycine max)	Correa, C. R.; Li, L.; Aldini, G.; Carini, M.; Oliver Chen, C. Y.; Chun, H.; Cho, S.; Park, K.; Russell, R. M.; Blumberg, J. B.; Yeum, K.	*Food Chem. 123 (4),* 1176–1184	2010 Dec 15
Effect of UV-B light and different cutting styles on antioxidant enhancement of commercial fresh-cut carrot products	Du, W.; Avena-Bustillos, R. J.; Breksa, A. P., III.; McHugh, T. H.	*Food Chem. 134 (4),* 1862–1869	2012 Oct 15

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Phenols, lignans and antioxidant properties of legume and sweet chestnut flours	Durazzo, A.; Turfani, V.; Azzini, E.; Maiani, G.; Carcea, M.	*Food Chem. 140 (4),* 666–671	2013 Oct 15
alpha-Lipoic acid in dietary supplements: development and comparison of HPLC-CEAD and HPLC-ESI-MS methods	Durrani, A. I.; Schwartz, H.; Schmid, W.; Sontag, G.	*J. Pharm. Biomed. Anal. 45 (4),* 694–699	2007 Nov 30
Comparison between evaporative light scattering detection and charged aerosol detection for the analysis of saikosaponins	Eom, H. Y.; Park, S. Y.; Kim, M. K.; Suh, J. H.; Yeom, H.; Min, J. W.; Kim, U.; Lee, J.; Youm, J. R.; Han, S. B.	*J. Chromatogr., A. 1217 (26),* 4347–4354	2010 Jun 25
Assessment of microcystin purity using charged aerosol detection	Edwards, C.; Lawton, L. A.	*J. Chromatogr., A. 1217 (32),* 5233–5238	2010 Aug 6
Analysis of lycopene geometrical isomers in biological microsamples by liquid chromatography with coulometric array detection	Ferruzzi, M. G.; Nguyen, M. L.; Sander, L. C.; Rock, C. L.; Schwartz, S. J.	*J. Chromatogr., B: Biomed. Sci. Appl. 760 (2),* 289–299	2001 Sep 5
Charged aerosol detection to characterize components of dispersed-phase formulations	Fox, C. B.; Sivananthan, S. J.; Mikasa, T. J.; Lin, S.; Parker, S. C.	*Adv. Colloid Interface Sci. 199–200,* 59–65	2013 Nov
HPLC with charged aerosol detection for the measurement of natural products	Fukushima, K.; Kanedai, Y.; Hirose, K.; Matsumoto, T.; Hashiguchi, K.; Senda, M.; et al.	*Chromatography 27 (Suppl. 1),* 83–86	2006
Determination of heterocyclic aromatic amines in beef extract, cooked meat and rat urine by liquid chromatography with coulometric electrode array detection	Gerbl, U.; Cichna, M.; Zsivkovits, M.; Knasmüller, S.; Sontag, G.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 802 (1),* 107–113	2004 Mar 25
Determination of macrolide antibiotics in porcine and bovine urine by high-performance liquid chromatography coupled to coulometric detection	González de la Huebra, M. J.; Vincent, U.; Bordin, G.; Rodríguez, A. R.	*Anal. Bioanal. Chem. 382 (2),* 433–439	2005 May
Development and validation of HPLC-DAD-CAD-MS3 method for qualitative and quantitative standardization of polyphenols in *Agrimoniae eupatoriae herba* (Ph. Eur)	Granica, S.; Krupa, K.; Kłębowska, A.; Kiss, A. K.	*J. Pharm. Biomed. Anal. 86,* 112–122	2013 Dec
Total reducing capacity of fresh sweet peppers and five different Italian pepper recipes	Greco, L.; Riccio, R.; Bergero, S.; Del Re, A. A. M.; Trevisan, M.	*Food Chem. 103 (4),* 1127–1133	2007 Jan
Urinary 3-(3,5-dihydroxyphenyl)-1-propanoic acid, an alkylresorcinol metabolite, is a potential biomarker of whole-grain intake in a U.S. population	Guyman, L. A.; Adlercreutz, H.; Koskela, A.; Li, L.; Beresford, S. A.; Lampe, J. W.	*J. Nutr. 138 (10),* 1957–1962	2008 Oct
Multidimensional LC x LC analysis of phenolic and flavone natural antioxidants with UV-electrochemical coulometric and MS detection	Hájek, T.; Skeríková, V.; Cesla, P.; Vynuchalová, K.; Jandera, P.	*J. Sep. Sci. 31 (19),* 3309–3328	2008 Oct
Determination of the urinary aglycone metabolites of vitamin K by HPLC with redox-mode electrochemical detection	Harrington, D. J.; Soper, R.; Edwards, C.; Savidge, G. F.; Hodges, S. J.; Shearer, M. J.	*J. Lipid Res. 46 (5),* 1053–1060	2005 May

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Bioavailability and antioxidant effect of epigallocatechin gallate administered in purified form versus as green tea extract in healthy individuals	Henning, S. M.; Niu, Y.; Liu, Y.; Lee, N. H.; Hara, Y.; Thames, G. D.; Minutti, R. R.; Carpenter, C. L.; Wang, H.; Heber, D.	*J. Nutr. Biochem. 16 (10),* 610–616	2005 Oct
Procyanidin dimer B_2 [epicatechin-(4beta-8)-epicatechin] in human plasma after the consumption of â flavanol-rich cocoa	Holt, R. R.; Lazarus, S. A.; Sullards, M. C.; Zhu, Q. Y.; Schramm, D. D.; Hammerstone, J. F.; Fraga, C. G.; Schmitz, H. H.; Keen, C. L.	*Am. J. Clin. Nutr. 76 (4),* 798–804	2002 Oct
Effects of natural (RRR α-tocopherol acetate) or synthetic (all-rac α-tocopherol acetate) vitamin E supplementation on reproductive efficiency in beef cows	Horn, M.; Gunn, P.; Van Emon, M.; Lemenager, R.; Burgess, J.; Pyatt, N. A.; Lake, S. L.	*J. Anim. Sci. (Savoy, IL, U.S.) 88 (9),* 3121–3127	2010 Sep
RP-HPLC analysis of phenolic compounds and flavonoids in beverages and plant extracts using a CoulArray detector	Jandera, P.; Skeifíková, V.; Rehová, L.; Hájek, T.; Baldriánová, L.; Skopová, G.; Kellner, V.; Horna, A.	*J. Sep. Sci. 28 (9–10),* 1005–1022	2005 Jun
A new application of charged aerosol detection in liquid chromatography for the simultaneous determination of polar and less polar ginsenosides in ginseng products	Jia, S.; Li, J.; Yunusova, N.; Park, J. H.; Kwon, S. W.; Lee, J.	*Phytochem. Anal. 24 (4),* 374–380	2013 Jul–Aug
A combination of aspirin and γ-tocopherol is superior to that of aspirin and α-tocopherol in anti-inflammatory action and attenuation of aspirin-induced adverse effects	Jiang, Q.; Moreland, M.; Ames, B. N.; Yin, X.	*J. Nutr. Biochem. 20 (11),* 894–900	2009 Nov
HPLC analysis of rosmarinic acid in feed enriched with aerial parts of *Prunella vulgaris* and its metabolites in pig plasma using dual-channel coulometric detection	Jirovský, D.; Kosina, P.; Myslínová, M.; Stýskala, J.; Ulrichová, J.; Simánek V.	*J. Agric. Food Chem. 55 (19),* 7631–7637	2007 Sep 19
Molar absorptivities and reducing capacity of pyranoanthocyanins and other anthocyanins	Jordheim, M.; Aaby, K.; Fossen, T.; Skrede, G.; Andersen, Ø. M.	*J. Agric. Food Chem. 55 (26),* 10591–10598	2007 Dec 26
Sensitive electrochemical detection method for alpha-acids, beta-acids and xanthohumol in hops (*Humulus lupulus L.*)	Kac, J.; Vovk, T.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 850 (1–2),* 531–537	2007 May 1
Determination of phenolic compounds and hydroxymethylfurfural in meads using high performance liquid chromatography with coulometric-array and UV detection	Kahoun, D.; Rezková, S.; Veskrnová, K.; Královský, J.; Holcapek, M.	*J. Chromatogr., A 1202 (1),* 19–33	2008 Aug 15
Analysis of terpene lactones in a Ginkgo leaf extract by high-performance liquid chromatography using charged aerosol detection	Kakigi, Y.; Mochizuki, N.; Icho, T.; Hakamatsuka, T.; Goda, Y.	*Biosci., Biotechnol., Biochem. 74 (3),* 590–594	2010
Linear aglycones are the substrates for glycosyltransferase DesVII in methymycin biosynthesis: analysis and implications	Kao, C.; Borisova, S.; Kim, H.; Liu, H.	*J. Am. Chem. Soc. 128 (17),* 5606–5607	2006 May 3

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Antioxidant-rich food intakes and their association with blood total antioxidant status and vitamin C and E levels in community-dwelling seniors from the Quebec longitudinal study NuAge	Khalil, A.; Gaudreau, P.; Cherki, M.; Wagner, R.; Tessier, D. M.; Fulop, T.; Shatenstein, B.	*Exp. Gerontol. 46 (6),* 475–481	2011 Jun
Certification of a pure reference material for the ginsenoside Rg1	Kim, D.; Chang, J.; Sohn, H.; Cho, B.; Ko, S.; Nho, K.; Jang, D.; Lee, S.	*Accredit. Qual. Assur. 15 (2),* 81–87	2009 Sep
Optimization of pressurized liquid extraction for spicatoside A in *Liriope platyphylla*	Kim, S. H.; Kim, H. K.; Yang, E. S.; Lee, K. Y.; Kim, S. D.; Kim, Y. C.; Sung, S. H.	*Sep. Purif. Technol. 71 (2),* 168–172	2010
Production of surfactin and iturin by *Bacillus licheniformis* N1 responsible for plant disease control activity	Kong, H. G.; Kim, J. C.; Choi, G. J.; Lee, K. Y.; Kim, H. J.; Hwang, E. C.; Moon, B. J.; Lee, S. W.	*Plant Pathol. J. 26 (2),* 170–177	2010
Transepithelial transport of microbial metabolites of quercetin in intestinal Caco-2 cell monolayers	Konishi, Y.	*J. Agric. Food Chem. 53 (3),* 601–607	2005 Feb 9
Absorption and bioavailability of artepillin C in rats after oral administration	Konishi, Y.; Hitomi, Y.; Yoshida, M.; Yoshioka, E.	*J. Agric. Food Chem. 53 (26),* 9928–9933	2005 Dec 28
Pharmacokinetic study of caffeic and rosmarinic acids in rats after oral administration	Konishi, Y.; Hitomi, Y.; Yoshida, M.; Yoshioka, E.	*J. Agric. Food Chem. 53 (12),* 4740–4746	2005 Jun 15
Intestinal absorption of *p*-coumaric and gallic acids in rats after oral administration	Konishi, Y.; Hitomi, Y.; Yoshioka, E.	*J. Agric. Food Chem. 52 (9),* 2527–2532	2004 May 5
Microbial metabolites of ingested caffeic acid are absorbed by the monocarboxylic acid transporter (MCT) in intestinal Caco-2 cell monolayers	Konishi, Y.; Kobayashi, S.	*J. Agric. Food Chem. 52 (21),* 6418–6424	2004 Oct 20
Transepithelial transport of rosmarinic acid in intestinal Caco-2 cell monolayers	Konishi, Y.; Kobayashi, S.	*Biosci., Biotechnol., Biochem. 69 (3),* 583–591	2005 Mar
Effects of various doses of selenite on stinging nettle (*Urtica dioica L.*)	Krystofova, O.; Adam, V.; Babula, P.; Zehnalek, J.; Beklova, M.; Havel, L.; Kizek, R.	*Int. J. Environ. Res. Public Health 7 (10),* 3804–3815	2010 Oct
Biofortified cassava increases β-carotene and vitamin A concentrations in the TAG-rich plasma layer of American women	La Frano, M. R.; Woodhouse, L. R.; Burnett, D. J.; Burri, B. J.	*Br. J. Nutr. 110 (2),* 310–320	2013 Jul 28
Chlorogenic acid is absorbed in its intact form in the stomach of rats	Lafay, S.; Gil-Izquierdo, A.; Manach, C.; Morand, C.; Besson, C.; Scalbert, A.	*J. Nutr. 136 (5),* 1192–1197	2006 May
Determination of 4-ethylcatechol in wine by high-performance liquid chromatography-coulometric electrochemical array detection	Larcher, R.; Nicolini, G.; Bertoldi, D.; Nardin, T.	*Anal. Chim. Acta 609 (2),* 235–240	2008 Feb 25
Determination of volatile phenols in wine using high-performance liquid chromatography with a coulometric array detector	Larcher, R.; Nicolini, G.; Puecher, C.; Bertoldi, D.; Moser, S.; Favaro, G.	*Anal. Chim. Acta 582 (1),* 55–60	2007 Jan 16

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Acute, quercetin-induced reductions in blood pressure in hypertensive individuals are not secondary to lower plasma angiotensin-converting enzyme activity or endothelin-1: nitric oxide	Larson, A.; Witman, M. A. H.; Guo, Y.; Ives, S.; Richardson, R. S.; Bruno, R. S.; Jalili, T.; Symons, J. D.	*Nutr. Res. (N. Y., NY, U.S.) 32 (8),* 557–564	2012 Aug
High-performance liquid chromatography method for the determination of folic acid in fortified food products	Lebiedzińska, A.; Dąbrowska, M.; Szefer, P.; Marszałł M.	*Toxicol. Mech. Methods 18 (6),* 463–467	2008 Jul
Reversed-phase high-performance liquid chromatography method with coulometric electrochemical and ultraviolet detection for the quantification of vitamins B(1) (thiamine), B(6) (pyridoxamine, pyridoxal and pyridoxine) and B(12) in animal and plant foods	Lebiedzińska, A.; Marszałł, M. L.; Kuta, J.; Szefer, P.	*J. Chromatogr., A 1173 (1–2),* 71–80	2007 Nov 30
An improved method for the determination of green and black tea polyphenols in biomatrices by high-performance liquid chromatography with coulometric array detection	Lee, M. J.; Prabhu, S.; Meng, X.; Li, C.; Yang, C. S.	*Anal. Biochem. 279 (2),* 164–169	2000 Mar 15
Characterisation, extraction efficiency, stability and antioxidant activity of phytonutrients in *Angelica keiskei*	Li, L.; Aldini, G.; Carini, M.; Chen, C. Y. O.; Chun, H.; Cho, S.; Park, K.; Correa, C. R.; Russell, R. M.; Blumberg, J. B.; Yeum, K.	*Food Chem.* 115 (1), 227–232	2009 Jul
Vitamin A equivalence of the β-carotene in β-carotene-biofortified maize porridge consumed by women	Li, S.; Nugroho, A.; Rocheford, T.; White, W. S.	*Am. J. Clin. Nutr. 92 (5),* 1105–1112	2010 Nov
Phase IIa chemoprevention trial of green tea polyphenols in high-risk individuals of liver cancer: modulation of urinary excretion of green tea polyphenols and 8-hydroxydeoxyguanosine	Luo, H.; Tang, L.; Tang, M.; Billam, M.; Huang, T.; Yu, J.; Wei, Z.; Liang, Y.; Wang, K.; Zhang, Z. Q.; Zhang, L.; Wang, J. S.	*Carcinogenesis 27 (2),* 262–268	2006 Feb
Determination of four water-soluble compounds in *Salvia miltiorrhiza Bunge* by high-performance liquid chromatography with a coulometric electrode array system	Ma, L.; Zhang, X.; Guo, H.; Gan, Y.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 833* (2), 260–263	2006 Apr 3
Effect of green tea powder (*Camellia sinensis L.* cv. Benifuuki) particle size on O-methylated EGCG absorption in rats, The Kakegawa Study	Maeda-Yamamoto, M.; Ema, K.; Tokuda, Y.; Monobe, M.; Tachibana, H.; Sameshima, Y.; Kuriyama, S.	*Cytotechnology 63 (2),* 171–179	2011 Mar
Supplementation of a γ-tocopherol-rich mixture of tocopherols in healthy men protects against vascular endothelial dysfunction induced by postprandial hyperglycemia	Mah, E.; Noh, S. K.; Ballard, K. D.; Park, H. J.; Volek, J. S.; Bruno, R. S.	*J. Nutr. Biochem. 24 (1),* 196–203	2013 Jan

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Mediterranean diet reduces endothelial damage and improves the regenerative capacity of endothelium	Marin, C.; Ramirez, R.; Delgado-Lista, J.; Yubero-Serrano, E. M.; Perez-Martinez, P.; Carracedo, J.; Garcia-Rios, A.; Rodriguez. F.; Gutierrez-Mariscal, F. M.; Gomez, P.; Perez-Jimenez, F.; Lopez-Miranda, J.	*Am. J. Clin. Nutr. 93 (2),* 267–274	2011 Feb
Photodiode array (PDA) and other detection methods in HPLC of plant metabolites	Markowski, W.; Waksmundzka-Hajnos, M.	Chapter 13 in *High Performance Liquid Chromatography in Phytochemical Analysis,* Chromatographic Science Series, Markowski, W., Sherma, J., Eds.; Taylor & Francis Group, LLC: Boca Raton, FL; 331–350	2010 Nov
Determination of water-soluble vitamins in infant milk and dietary supplement using a liquid chromatography on-line coupled to a corona-charged aerosol detector	Márquez-Sillero, I.; Cárdenas, S.; Valcárcel, M.	*J. Chromatogr., A. 1313C,* 253–258	2013 Oct 25
Sensitive high-performance liquid chromatographic method using coulometric electrode array detection for measurement of phytoestrogens in dried blood spots	Melby, M. K.; Watanabe, S.; Whitten, P. L.; Worthman, C. M.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 826 (1–2),* 81–90	2005 Nov 5
Phenolic acids from beer are absorbed and extensively metabolized in humans	Nardini, M.; Natella, F.; Scaccini, C.; Ghiselli, A.	*J. Nutr. Biochem. 17 (1),* 14–22	2006 Jan
High-performance liquid chromatography analysis of plant saponins: An update 2005-2010	Negi, J. S.; Singh, P.; Pant, G. J.; Rawat, M. S.	*Pharmacogn. Rev. 5 (10),* 155–158	2011 Jul
Physicochemical effect of pH and antioxidants on mono- and triglutamate forms of 5-methyltetrahydrofolate, and evaluation of vitamin stability in human gastric juice: Implications for folate bioavailability	Ng, X.; Lucock, M.; Veysey, M.	*Food Chem. 106 (1),* 200–210	2008 Jan
Practical preparation of lacto-*N*-biose I, a candidate for the bifidus factor in human milk	Nishimoto, M.; Kitaoka, M.	*Biosci., Biotechnol., Biochem. 71 (8),* 2101-2104	2007 Aug
Hydrophilic interaction liquid chromatography—charged aerosol detection as a straightforward solution for simultaneous analysis of ascorbic acid and dehydroascorbic acid	Nováková, L.; Solichová, D.; Solich, P.	*J. Chromatogr., A. 1216 (21),* 4574–4581	2009 May 22

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
No effect on adenoma formation in Min mice after moderate amount of flaxseed	Oikarinen, S.; Heinonen, S. M.; Nurmi, T.; Adlercreutz, H.; Mutanen, M.	*Eur. J. Nutr. 44 (5),* 273–280	2005 Aug
Measurement of isoflavones using liquid chromatography with multi-channel coulometric electrochemical detection	Ouchi, K.; Gamache, P.; Acworth, I.; Watanabe, S.	*BioFactors. 22 (1–4),* 353–356	2004
Quantitation of clovamide-type phenylpropenoic acid amides in cells and plasma using high-performance liquid chromatography with a coulometric electrochemical detector	Park, J. B.	*J. Agric. Food Chem. 53 (21),* 8135–8140	2005 Oct 19
Synthesis, HPLC measurement and bioavailability of the phenolic amide amkamide	Park, J. B.	*J. Chromatogr. Sci.* [Epub ahead of print]	2013 May 27
Synthesis of safflomide and its HPLC measurement in mouse plasma after oral administration	Park, J. B.; Chen, P.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci.* 852 (1–2), 398–402	2007 Jun 1
Determination of lignans in human plasma by liquid chromatography with coulometric electrode array detection	Peñalvo, J. L.; Nurmi, T.; Haajanen, K.; Al-Maharik, N.; Botting, N.; Adlercreutz, H.	*Anal. Biochem. 332 (2),* 384–393	2004 Sep 15
Supercritical antisolvent fractionation of lignans from the ethanol extract of flaxseed	Perretti, G.; Virgili, C.; Troilo, A.; Marconi, O.; Regnicoli, G. F.; Fantozzi, P.	*J. Supercrit. Fluids 75,* 94–100	2013 Mar
Analysis of flavonoids in honey by HPLC coupled with coulometric electrode array detection and electrospray ionization mass spectrometry	Petrus, K.; Schwartz, H.; Sontag, G.	*Anal. Bioanal. Chem. 400 (8),* 2555–2563	2011 Jun
High-dose supplementation with natural α-tocopherol does neither alter the pharmacodynamics of atorvastatin nor its phase I metabolism in guinea pigs	Podszun, M. C.; Grebenstein, N.; Hofmann, U.; Frank, J.	*Toxicol. Appl. Pharmacol. 266 (3),* 452–458	2013 Feb 1
Application of high-performance liquid chromatography with charged aerosol detection for universal quantitation of undeclared phosphodiesterase-5 inhibitors in herbal dietary supplements	Poplawska, M.; Blazewicz, A.; Bukowinska, K.; Fijalek, Z.	*J. Pharm. Biomed. Anal. 84,* 232–243	2013 Oct
Isolation and analysis of ginseng: advances and challenges	Qi, L.; Wang, C.; Yuan, C.	*Nat. Prod. Rep. 28 (3),* 467–495	2011 Mar
Folate analysis in complex food matrices: Use of a recombinant Arabidopsis γ-glutamyl hydrolase for folate deglutamylation	Ramos-Parra, P. A.; Urrea-López, R.; Díaz de la Garza, R. I.	*Food Res. Int. 54 (1),* 177–185	2013 Nov
Optimisation of gradient HPLC analysis of phenolic compounds and flavonoids in beer using a coularray detector	Rehová, L.; Skeríková, V.; Jandera, P.	*J. Sep. Sci. 27 (15–16),* 1345–1359	2004 Nov
Chiral separation of (+)/(-)-catechin from sulfated and glucuronidated metabolites in human plasma after cocoa consumption	Ritter, C.; Zimmermann, B. F.; Galensa, R.	*Anal. Bioanal. Chem. 397 (2),* 723–730	2010 May

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Analysis of alkylresorcinols in cereal grains and products using ultrahigh-pressure liquid chromatography with fluorescence, ultraviolet, and CoulArray electrochemical detection	Ross, A. B.	*J. Agric. Food Chem. 60 (36),* 8954–8962	2012 Sep 12
Rapid and sensitive analysis of alkylresorcinols from cereal grains and products using HPLC-CoulArray-based electrochemical detection	Ross, A. B.; Kochhar, S.	*J. Agric. Food Chem. 57 (12),* 5187–5193	2009 Jun 24
Analysis of soy isoflavone plasma levels using HPLC with coulometric detection in postmenopausal women	Saracino, M. A.; Raggi, M. A.	*J. Pharm. Biomed. Anal. 53 (3),* 682–687	2010 Nov 2
A biosynthetic pathway for BE-7585A, a 2-thiosugar-containing angucycline-type natural product	Sasaki, E.; Ogasawara, Y.; Liu, H. W.	*J. Am. Chem. Soc. 132 (21),* 7405–7417	2010 Jun 2
The senescence-accelerated mouse-prone 8 is not a suitable model for the investigation of cardiac inflammation and oxidative stress and their modulation by dietary phytochemicals	Schiborr, C.; Schwamm, D.; Kocher, A.; Rimbach, G.; Eckert, G. P.; Frank, J.	*Pharmacol. Res. 74,* 113–120	2013 Aug
Comprehensive impurity profiling of nutritional infusion solutions by multidimensional off-line reversed-phase liquid chromatography × hydrophilic interaction chromatography-ion trap mass-spectrometry and charged aerosol detection with universal calibration	Schiesel, S.; Lämmerhofer, M.; Lindner, W.	*J. Chromatogr., A. 1259,* 100–10	2012 Oct 12
The effect of α-tocopherol supplementation on training-induced elevation of S100B protein in sera of basketball players	Schulpis, K. H.; Moukas, M.; Parthimos, T.; Tsakiris, T.; Parthimos, N.; Tsakiris, S.	*Clin. Biochem. 40 (12),* 900–906	2007 Aug
Determination of secoisolariciresinol, lariciresinol and isolariciresinol in plant foods by high performance liquid chromatography coupled with coulometric electrode array detection	Schwartz, H.; Sontag, G.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci.* 838 (2), 78–85	2006 Jul 11
Assessment of probiotic strains ability to reduce the bioaccessibility of aflatoxin M 1 in artificially contaminated milk using an in vitro digestive model	Serrano-Niño, J. C.; Cavazos-Garduño, A.; Hernandez-Mendoza, A.; Applegate, B.; Ferruzzi, M. G.; San Martin-González, M. F.; García, H. S.	*Food Control 31 (1),* 202–207	2013 May
Intestinal uptake of quercetin-3-glucoside in rats involves hydrolysis by lactase phlorizin hydrolase	Sesink, A. L.; Arts, I. C.; Faassen-Peters, M.; Hollman, P. C.	*J. Nutr. 133 (3),* 773–776	2003 Mar
Quercetin glucuronides but not glucosides are present in human plasma after consumption of quercetin-3-glucoside or quercetin-4'-glucoside	Sesink, A. L.; O'Leary, K. A.; Hollman, P. C.	*J. Nutr. 131 (7),* 1938–1941	2001 Jul
Co-administration of quercetin and catechin in rats alters their absorption but not their metabolism	Silberberg, M.; Morand, C.; Manach, C.; Scalbert, A.; Remesy, C.	*Life Sci. 77 (25),* 3156–3167	2005 Nov 4
Nutritional status is altered in the self-neglecting elderly	Smith, S. M.; Mathews Oliver, S. A.; Zwart, S. R.; Kala, G.; Kelly, P. A.; Goodwin, J. S.; Dyer, C. B.	*J. Nutr. 136 (10),* 2534–2541	2006 Oct

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Binding of heterocyclic aromatic amines by lactic acid bacteria: results of a comprehensive screening trial	Stidl, R.; Sontag, G.; Koller, V.; Knasmüller, S.	*Mol. Nutr. Food Res. 52 (3),* 322–329	2008 Mar
Direct separation and detection of biogenic amines by ion-pair liquid chromatography with chemiluminescent nitrogen detector	Sun, J.; Guo, H. X.; Semin, D.; Cheetham, J.	*J. Chromatogr., A. 1218 (29),* 4689–4697	2011 Jul 22
Rapid purification method for fumonisin B1 using centrifugal partition chromatography	Szekeres, A.; Lorántfy, L.; Bencsik, O.; Kecskeméti, A.; Szécsi, Á.; Mesterházy, Á.; Vágvölgyi, C.	*Food Addit. Contam. 30 (1),* 147–155	2013
Determination of coenzyme Q10 in over-the-counter dietary supplements by high-performance liquid chromatography with coulometric detection	Tang, P. H.	*J. AOAC Int. 89 (1),* 35–39	2006 Jan–Feb
α-Tocopherol supplementation restores the reduction of erythrocyte glucose-6-phosphate dehydrogenase activity induced by forced training	Tsakiris, S.; Reclos, G. J.; Parthimos, T.; Tsakiris, T.; Parthimos, N.; Schulpis, K. H.	*Pharmacol. Res. 54 (5),* 373–379	2006 Nov
Tissue distribution of isoflavones in ewes after consumption of red clover silage	Urpi-Sarda, M.; Morand, C.; Besson, C.; Kraft, G.; Viala, D.; Scalbert, A.; Besle, J. M.; Manach, C.	*Arch. Biochem. Biophys. 476 (2),* 205–210	2008 Aug 15
Performance evaluation of charged aerosol and evaporative light scattering detection for the determination of ginsenosides by LC	Wang, L.; He, W. S.; Yan, H. X.; Jiang, Y.; Bi, K. S.; Tu, P. F.	*Chromatographia 70 (3–4),* 603–608	2009 Aug
Catechins are bioavailable in men and women drinking black tea throughout the day	Warden, B. A.; Smith, L. S.; Beecher, G. R.; Balentine, D. A.; Clevidence, B. A.	*J. Nutr. 131 (6),* 1731–1737	2001 Jun
Identification and quantification of polyphenol phytoestrogens in foods and human biological fluids	Wilkinson, A. P.; Wähälä, K.; Williamson, G.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 777 (1–2),* 93–109	2002 Sep 25
Bioavailability and pharmacokinetics of caffeoylquinic acids and flavonoids after oral administration of Artichoke leaf extracts in humans	Wittemer, S. M.; Ploch, M.; Windeck, T.; Müller, S. C.; Drewelow, B.; Derendorf, H.; Veit, M.	*Phytomedicine 12 (1–2),* 28–38	2005 Jan
Validated method for the determination of six metabolites derived from artichoke leaf extract in human plasma by high-performance liquid chromatography-coulometric-array detection	Wittemer, S. M.; Veit, M.	*J. Chromatogr., B: Anal. Technol. Biomed. Life Sci. 793 (2),* 367–375	2003 Aug 15
HPLC in natural product analysis: The detection issue	Wolfender, J. L.	*Planta Med. 75 (07),* 719–734	2009 Jun
Simultaneous determination of isoflavones and bisphenol A in rat serum by high-performance liquid chromatography coupled with coulometric array detection	Yasuda, S.; Wu, P. S.; Hattori, E.; Tachibana, H.; Yamada, K.	*Biosci., Biotechnol., Biochem. 68 (1),* 51–58	2004 Jan
Impurities from polypropylene microcentrifuge tubes as a potential source of interference in simultaneous analysis of multiple lipid-soluble antioxidants by HPLC with electrochemical detection	Yen, H. C.; Hsu, Y. T.	*Clin. Chem. Lab. Med. 42 (4),* 390–395	2004 Apr

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Food, Nutrition, Natural Products, and Supplements

Title	Authors	Publication	Publication Date
Simultaneous determination of triterpenoid saponins from *pulsatilla koreana* using high performance liquid chromatography coupled with a charged aerosol detector (HPLC-CAD)	Yeom, H.; Suh, J. H.; Youm, J. R.; Han, S. B.	*Bull. Korean Chem. Soc. 31 (5),* 1159–1164	2010
DPPH radical scavenging activities of 31 flavonoids and phenolic acids and 10 extracts of Chinese materia medica	Yuan, Y.; Chen, C.; Yang, B.; Kusu, F.; Kotani, A.	*Zhongguo Zhongyao Zazhi 34 (13),* 1695–1700	2009 Jul
Determination of residual clenbuterol in pork meat and liver by HPLC with electrochemical detection	Zhang, X. Z.; Gan, Y. R.; Zhao, F. N.	*Yaoxue Xuebao 39 (4),* 276–280	2004 Apr
Identification of equol producers in a Japanese population by high-performance liquid chromatography with coulometric array for determining serum isoflavones	Zhao, J. H.; Sun, S. J.; Arao, Y.; Oguma, E.; Yamada, K.; Horiguchi, H.; Kayama, F.	*Phytomedicine 13 (5),* 304–309	2006 May
Simultaneous sampling of volatile and non-volatile analytes in beer for fast fingerprinting by extractive electrospray ionization mass spectrometry	Zhu, L.; Hu, Z.; Gamez, G.; Law, W. S.; Chen, H.; Yang, S.; Chingin, K.; Balabin, R. M.; Wang, R.; Zhang, T.; Zenobi, R.	*Anal. Bioanal. Chem. 398 (1),* 405–413	2010 Sep
Comparison of various easy-to-use procedures for extraction of phenols from apricot fruits	Zitka, O.; Sochor, J.; Rop, O.; Skalickova, S.; Sobrova, P.; Zehnalek, J.; Beklova, M.; Krska, B.; Adam, V.; Kizek, R.	*Molecules 16 (4),* 2914–2936	2011 Apr 4

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Lipids

Title	Authors	Publication	Publication Date
Development of analytical procedures to study changes in the composition of meat phospholipids caused by induced oxidation	Cascone, A.; Eerola, S.; Ritieni, A.; Rizzo, A.	*J. Chromatogr., A 1120 (1–2),* 211–220	2006 Jul 7
Evaporative light scattering and charged aerosol detector.	Chaminade, P.	Chapter 5. In *Hyphenated and Alternative Methods of Detection in Chromatography,* Chromatographic Science Series; Shalliker, A., Ed.; Taylor & Francis Group, LLC: Boca Raton, FL.; 145–160	2012
Simple and efficient profiling of phospholipids in phospholipase D-modified soy lecithin by HPLC with charged aerosol detection	Damnjanovic´, J.; Nakano, H.; Iwasaki, Y.	*J. Am. Oil Chem. Soc. 90 (7),* 951–957	2013 Jul
Discriminating olive and non-olive oils using HPLC-CAD and chemometrics	de la Mata-Espinosa, P.; Bosque-Sendra, J. M.; Bro, R.; Cuadros-Rodríguez, L.	*Anal. Bioanal. Chem. 399 (6),* 2083–2092	2011 Feb
Olive oil quantification of edible vegetable oil blends using triacylglycerols chromatographic fingerprints and chemometric tools	de la Mata-Espinosa, P.; Bosque-Sendra, J. M.; Bro, R.; Cuadros-Rodríguez, L.	*Talanta 85 (1),* 177–182	2011 Jul 15
Quantification of triacylglycerols in olive oils using HPLC-CAD	de la Mata-Espinosa, P.; Bosque-Sendra, J.; Cuadros-Rodriguez, L.	*Food Analytical Methods 4 (4), 574–581*	2011 Dec
Quantification of pegylated phospholipids decorating polymeric microcapsules of perfluorooctyl bromide by reverse phase HPLC with a charged aerosol detector	Díaz-López, R.; Libong, D.; Tsapis, N.; Fattal, E.; Chaminade, P.	*J. Pharm. Biomed. Anal. 48 (3),* 702–707	2008 Nov 4
Squalene emulsions for parenteral vaccine and drug delivery	Fox, C. B.	*Molecules 14 (9),* 3286–3312	2009 Sep 1
Interactions between parenteral lipid emulsions and container surfaces	Gonyon, T.; Tomaso, A.; Kotha, P.; Owen, H.; Patel, D.; Carter, P.; Cronin, J.; Green, J.	*PDA J. Pharm. Sci. and Tech. 67 (3),* 247–254	2013 May–Jun
Composition analysis of positional isomers of phosphatidylinositol by high-performance liquid chromatography	Iwasaki, Y.; Masayama, A.; Mori, A.; Ikeda, C.; Nakano, H.	*J. Chromatogr., A 1216 (32),* 6077–6080	2009 Aug 7
Determination of phospholipid and its degradation products in liposomes for injection by HPLC-charged aerosol detection (CAD)	Jiang, Q.; Yang, R.; Mei, X.	*Chinese Pharmaceutical Journal (Zhongguo Yaoxue Zazhi, Beijing, China) 42 (23),* 1794–1796	2007

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Lipids

Title	Authors	Publication	Publication Date
Rapid quantification of yeast lipid using microwave-assisted total lipid extraction and HPLC-CAD	Khoomrung, S.; Chumnanpuen, P.; Jansa-Ard, S.; Ståhlman, M.; Nookaew, I.; Borén, J.; Nielsen, J.	*Anal. Chem. 85 (10),* 4912–4919	2013 May 21
A new liquid chromatography method with charge aerosol detector (CAD) for the determination of phospholipid classes. Application to milk phospholipids	Kieibowicz, G.; Micek, P.; Wawrzenczyk, C.	*Talanta 105,* 28–33	2013 Feb 15
An LC method for the analysis of phosphatidylcholine hydrolysis products and its application to the monitoring of the acyl migration process	Kiełbowicz, G.; Smuga, D.; Gładkowski, W.; Chojnacka, A.; Wawrzeńczyk, C.	*Talanta 94,* 22–29	2012 May 30
Separation of acylglycerols, FAME and FFA in biodiesel by size exclusion chromatography	Kittirattanapiboon, K.; Krisnangkurá, K.	*Eur. J. Lipid Sci. Technol. 110 (5),* 422–427	2008 Mar 17
Quantitation of triacylglycerols from plant oils using charged aerosol detection with gradient compensation	Lísa, M.; Lynen, F.; Holčapek, M.; Sandra, P.	*J. Chromatogr., A. 1176 (1–2),* 135–142	2007 Dec 28
Quantitative study of the stratum corneum lipid classes by normal phase liquid chromatography: comparison between two universal detectors	Merle, C.; Laugel, C.; Chaminade, P.; Baillet-Guffroy, A.	*J. Liq. Chromatogr. Relat. Technol. 33,* 629–644	2010 Mar
The analysis of lipids via HPLC with a charged aerosol detector	Moreau, R. A.	*Lipids 41 (7),* 727–34	2006 Jul
Lipid analysis via HPLC with a charged aerosol detector	Moreau, R. A.	*Lipid Technol. 21* (8–9), 191–194	2009 Oct 23
Extraction and analysis of food lipids	Moreau, R. A.; Winkler-Moser, J. K.	Chapter 6 in *Methods of Analysis of Food Components and Additives,* Second Edition; Ötles, S., Ed.; Taylor & Francis Group, LLC: Boca Raton, FL.; 115–134	2011 Nov
Aerosol based detectors for the investigation of phospholipid hydrolysis in a pharmaceutical suspension formulation	Nair, L.; Werling, J.	*J. Pharm. Biomed. Anal. 49 (1),* 95–99	2009 Jan 15
Structure/function relationships of adipose phospholipase A2 containing a cys-his-his catalytic triad	Pang, X. Y.; Cao, J.; Addington, L.; Lovell, S.; Battaile, K. P.; Zhang, Rao, J. L.; Dennis, E. A.; Moise, A. R.	*J. Biol. Chem. 287 (42),* 35260–35274	2012 Oct 12
Simultaneous assessment of lipid classes and bile acids in human intestinal fluid by solid-phase extraction and HPLC methods	Persson, E.; Löfgren, L.; Hansson, G.; Abrahamsson, B.; Lennernäs, H.; Nilsson, R.	*J. Lipid Res. 48 (1),* 242–251	2007 Jan

Thermo SCIENTIFIC

Peer Reviewed Journals: HPLC and UHPLC Methods

Lipids

Title	Authors	Publication	Publication Date
The use of charged aerosol detection with HPLC for the measurement of lipids	Plante, M.; Bailey, B.; Acworth, I.	*Methods Mol. Biol.* (Totowa, NJ, U.S.) 579, 469–482	2009
Comparison between charged aerosol detection and light scattering detection for the analysis of Leishmania membrane phospholipids	Ramos, R. G.; Libong, D.; Rakotomanga, M.; Gaudin, K.; Loiseau, P. M.; Chaminade, P.	*J. Chromatogr., A. 1209 (1–2),* 88–94	2008 Oct 31
Authentication of geographical origin of palm oil by chromatographic fingerprinting of triacylglycerols and partial least square-discriminant analysis	Ruiz-Samblás, C.; Arrebola-Pascual, C.; Tres, A.; van Ruth, S.; Cuadros-Rodríguez, L.	*Talanta. 116,* 788–793	2013 Nov 15
Simple and precise detection of lipid compounds present within liposomal formulations using a charged aerosol detector	Schönherr, C.; Touchene, S.; Wilser, G.; Peschka-Süss, R.; Francese, G.	*J. Chromatogr., A. 1216 (5),* 781–786	2009 Jan 30
Determination of intralumenal individual bile acids by HPLC with charged aerosol detection	Vertzoni, M.; Archontaki, H.; Reppas, C.	*J. Lipid Res. 49 (12),* 2690–2695	2008 Dec
Neurolipids and the use of a charged aerosol detector	Waraska, J.; Acworth, I.	*Am. Biotechnol. Lab. 26 (1),* 12–13	2008

Thermo SCIENTIFIC

Technical Collateral: HPLC and UHPLC Methods

Product Number	Technique	Title
AB 119	UV	Rapid Separation of Paclitaxel and Related Compounds in Paclitaxel Injection
AB 134	MS	LC-MS Analysis of Anthocyanins in Bilberry Extract
AB 139	UV	Separation of Schizandrin, Schizandrin A, and Schizandrin B in a Tablet Sample
AB 153	UV	Save the Flavor – Robust Iso-α-Acids Assaying in Beer within Ten Minutes
AB 155	UV	Monitor the Brewing Process with LC-Transformation of Hop alpha-Acids into Beer Iso-alpha-Acids
AN 109	FLD	Determination of Glyphosate by Cation-Exchange Chromatography with Postcolumn Derivatization
AN 156	UV	The Everlasting Paradigm-Keep Beer Tradition or Prevent Beer from a Skunky Off-Flavor?
AN 196	FLD	Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in Edible Oils by Donor-Acceptor Complex Chromatography (DACC)-HPLC with Fluorescent Detection
AN 207	UV	Chromatographic Fingerprinting of *Flos Chrysanthema indici* Using HPLC
AN 213	UV/FLD	Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in Tap Water Using on-Line Solid-Phase Extraction Followed by HPLC with UV and Fluorescence Detections
AN 216	UV	Determination of Water- and Fat-Soluble Vitamins in Functional Waters by HPLC with UV-PDA Detection
AN 224	UV	Determination of Melamine in Milk Powder by Reversed-Phase HPLC with UV Detection
AN 232	UV	Determination of Anthraquinones and Stilbenes in Giant Knotweed Rhizome by HPLC with UV Detection
AN 236	UV	Determination of Iodide and Iodate in Seawater and Iodized Table Salt by HPLC-UV Detection
AN 245	UV	Fast Analysis of Dyes in Foods and Beverages
AN 251	UV	Determination of Water- and Fat-Soluble Vitamins in Nutritional Supplements by HPLC with UV Detection
AN 252	UV	HPLC Assay of Water-Soluble Vitamins, Fat-Soluble Vitamins, and a Preservative in Dry Syrup Multivitamin Formulation
AN 261	UV	Sensitive Determination of Microcystins in Drinking and Environmental Waters
AN 264	UV	Fast Determination of Anthocyanins in Pomegranate Juice
AN 266	FLD	Determination of Sialic Acids Using UHPLC with Fluorescence Detection
AN 272	FLD	Faster Yet Sensitive Determination of N-Methylcarbamates in Rice, Potato, and Corn by HPLC
AN 275	UV	Sensitive Determination of Catechins in Tea by HPLC
AN 287	UV	Two-Dimensional HPLC Combined with On-Line SPE for Determination of Sudan Dyes I–IV in Chili Oil
AN 292	UV	Determination of Aniline and Nitroanilines in Environmental and Drinking Waters by On-Line SPE
AN 293	CAD and UV	Steviol Glycoside Determination by HPLC with Charged Aerosol and UV Detections Using the Acclaim Trinity P1 Column
AN 299	UV	HPLC Analysis of Six Active Components of *Caulis Ionicerae* Using a Phenyl-1 Column
AN 1008	UV	Determination of Nitidine Chloride, Toddalolactone, and Chelerythrine Chloride by HPLC

Thermo SCIENTIFIC

Technical Collateral: HPLC and UHPLC Methods

Product Number	Technique	Title
AN 1020	EC, UV	Chalcinoids and Bitter Acids in Beer by HPLC with UV and ECD
AN 1023	UV	Determination of Sudan Dyes I–IV in Curry Paste
AN 1026	CAD	Fatty Acid Esters at Low Nanogram Levels
AN 1027	CAD	Ginseng
AN 1028	CAD	Ginkgo biloba
AN 1029	CAD	Black Cohosh
AN 1030	CAD	Soy Saponins
AN 1032	CAD	Unsaturated Fatty Acid: Arachidonic, Linoleic, Linolenic and Oleic Acids
AN 1033	CAD	Corn Syrup
AN 1034	CAD	Honey Sugars
AN 1035	CAD	Phenolic Acids
AN 1036	CAD	Water-Soluble Antioxidants: Ascorbic Acid, Glutathione and Uric Acid
AN 1037	CAD	Artificial Sweeteners-Global Method
AN 1039	CAD	Simultaneous Measurement of Glycerides (Mono-, Di- and Triglycerides) and Free Fatty Acids in Palm Oil
AN 1040	CAD	Analysis of Commercially Available Products Containing Stevia
AN 1041	CAD	Phytosterols
AN 1042	UV	Rapid Separation of Anthocyanins in Cranberry and Bilberry Extracts Using a Core-Shell Particle Column
AN 1045	UV	Determination of Phthalates in Drinking Water by UHPLC with UV Detection
AN 1046	UV	Determination of Phenylurea Compounds in Tap Water and Bottled Green Tea
AN 1055	CAD	Determination of Virginiamycin, Erythromycin, and Penicillin in Dried Distillers Grains with Solubles
AN 1063	ECD	Targeted Analyses of Secondary Metabolites in Herbs, Spices, and Beverages Using a Novel Spectro-Electro Array Platform
AN 1064	ECD	Product Authentication and Adulteration Determination Using a Novel Spectro-Electro Array Platform
AN 1067	UV	Determination of Carbendazim in Orange Juice
AN 1069	UV	Two-Dimensional HPLC Determination of Water-Soluble Vitamins in a Nutritional Drink
AN 1070	UV	Determination of Inositol Phosphates in Dried Distillers Grains and Solubles
AN 20583	UV	Determination of Catechins and Phenolic Acids in Red Wine by Solid Phase Extraction and HPLC
AN 20610	UV	Fast Analysis of Coffee Bean Extracts Using a Solid Core HPLC Column
AN 20663	CAD	Comparative Analysis of Cooking Oils Using a Solid Core HPLC Column
AN 20847	CAD	Analysis of a Sports Beverage for Electrolytes and Sugars Using Multi-Mode Chromatography with Charged Aerosol Detection

Thermo SCIENTIFIC

Technical Collateral: HPLC and UHPLC Methods

Product Number	Technique	Title
AN 70158	CAD	Novel Universal Approach for the Measurement of Natural Products in a Variety of Botanicals and Supplements
AN 70277	CAD	Simultaneous Analysis of Glycerides and Fatty Acids in Palm Oil
AU 144	UV	Determination of Hexavalent Chromium in Drinking Water Using Ion Chromatography
AU 170	UV	Fast Determination of Vanillin and its Synthesis Precursor by HPLC
AU 182	CAD	Measuring Lactose in Milk: A Validated Method
AU 184	CAD, UV	Mogroside V Determination by HPLC with Charged Aerosol and UV Detections
CAN 106	UV	Determination of the Punicalagins Found in Pomegranate by High Performance Liquid Chromatography
CAN 111	CAD	Determination of Triterpenes in *Centella asiatica* (Gotu Kola) by HPLC-CAD
CAN 112	CAD	Determination of Ginsenosides in Panax ginseng by HPLC-CAD
CAN 115	FLD	Clean-Up and Analysis of Aflatoxins and Ochratoxin A in Herbs and Spices
LPN 2062	MS	Profiling Analysis of 15 Prominent Naturally Occurring Phenolic Acids by LC-MS
LPN 2069	FLD	Fast and Effective Determination of Aflatoxins in Grains or Food Using Accelerated Solvent Extraction followed by HPLC
LPN 2421	UV	Achieving Maximum Productivity by Combining UHPLC with Advanced Chromatographic Techniques
LPN 2818	CAD	Analysis of Fat-Soluble Vitamins and Antioxidants in Supplements by RP-HPLC
LPN 2870	FLD	Benefits of High-Speed Wavelength Switching in UHPLC Methods Using Fluorescence Detection
LPN 2930	CAD	Determination of the Composition of Natural Products by HPLC with Charged Aerosol Detection
LPN 2923	CAD	Simple and Direct Analysis of Falcarinol and Other Polyacetylenic Oxylipins in Carrots by Reversed-Phase HPLC and Charged Aerosol Detection
LPN 2931	CAD	Quantification of Underivatized Omega-3 and Omega-6 Fatty Acids in Foods by HPLC CAD
LPN 2932	ECD	A Versatile Detector for the Sensitive and Selective Measurement of Numerous Fat-Soluble Vitamins and Antioxidants in Human Plasma and Plant Extracts
LPN 2934	CAD	Sensitive Analysis of Commonly Used Artificial and Natural Sweeteners Including Stevia and Their Impurities and Degradation Products
LPN 2991	CAD	Evaluation of Methods for the Characterization and Quantification of Polysorbates and Impurities Along with Other Surfactants and Emulsifiers Used in the Food and Pharmaceutical Industries
PN 70026	CAD	Carbohydrate Analysis Using PAD, FLD, CAD and MS Detectors
PN 70037	CAD	Sensitive HPLC Method for Triterpenoid Analysis Using Charged Aerosol Detection with Improved Resolution
PN 70055	CAD	Direct Analysis of Surfactants using HPLC with Charged Aerosol Detection
PN 70138	UV	Rapid Determination of Polyphenol Antioxidants in Green Tea and Cranberry Extract Using Core Shell Columns
PN 70538	CAD	Analysis of Silicone Oils by HPLC-CAD
PN 70540	CAD, ECD	Profiling *Hoodia* Extracts by HPLC with CAD, ECD, Principal Component Analysis

Thermo SCIENTIFIC

Table of Contents

References

Ion Chromatography References

Thermo SCIENTIFIC

Technical Collateral: Ion Chromatography Methods

Product Number	Technique	Title
AB 127	IC-PAD	Determination of Carbohydrates in Fruit Juice Using Capillary High-Performance Anion-Exchange Chromatography
AB 135	IC-SC	Determination of Anions and Organic Acids in Brewed Coffee Samples Using Capillary IC
AB 137	IC-SC	Determination of Inorganic and Organic Acids in Apple and Orange Juice Samples Using Capillary IC
AN 25	IC-SC	Determination of Inorganic Ions and Organic Acids in Non-Alcoholic Carbonated Beverages
AN 37	IC-PAD	Determination of Iodide and Iodate in Soy- and Mil-Based Infant Formulas
AN 46	IC-PAD	Ion Chromatography: A Versatile Technique for the Analysis of Beer
AN 54	IC-PAD	Determination of Total and Free Sulfite in Foods and Beverages
AN 67	IC-PAD	Determination of Plant-Derived Neutral Oligo- and Polysaccharides
AN 81	IC-SC	Ion Chromatographic Determination of Oxyhalides and Bromide at Trace Level Concentrations in Drinking Water Using direct Injection
AN 82	IC-PAD	Analysis of Fruit Juice Adulterated with Medium Invert Sugar from Beets
AN 87	IC-PAD	Determination of Sugar Alcohols in Confections and Fruit Juices by High-Performance Anion-Exchange Chromatography with Pulsed Amperometric Detection
AN 101	IC-SC	Trace Level Determination of Bromate in Ozonated Drinking Water Using Ion Chromatography
AN 112	IC-UV	Determination of Nitrate and Nitrite in Meat Using High-Performance Anion-Exchange Chromatography
AN 121	IC-SC	Analysis of Low Concentrations of Perchlorate in Drinking Water and Ground Water by Ion Chromatography
AN 123	IC-SC	Determination of Inorganic Anions and Organic Acids in Fermentation Broths
AN 133	IC-SC	Determination of Inorganic Anions in Drinking Water by Ion Chromatography
AN 136	IC-SC and IC-UV	Determination of Inorganic Oxyhalide Disinfection Byproduct Anions and Bromide in Drinking Water Using Ion Chromatography with the Addition of a Postcolumn Reagent for Trace Bromate Analysis
AN 140	IC-SC	Fast Analysis of Anions in Drinking Water by Ion Chromatography
AN 143	IC-SC	Determination of Organic Acids in Fruit Juices
AN 149	IC-SC	Determination of Chlorite, Bromate, Bromide, and Chlorate in Drinking Water by Ion Chromatography with an On-Line-Generated Postcolumn Reagent for Sub-µg/L Bromate Analysis
AN 150	IC-PAD	Determination of Amino Acids in Cell Cultures and Fermentation Broths
AN 154	IC-SC	Determination of Inorganic Anions in Environmental Waters Using a Hydroxide-Selective Column
AN 155	IC-PAD	Determination of Trans-Galactooligosaccharides in Foods by AOAC Method 2001.02

Thermo SCIENTIFIC

Technical Collateral: Ion Chromatography Methods

Product Number	Technique	Title
AN 165	IC-SC	Determination of Benzoate in Liquid Food Products by Reagent-Free Ion Chromatography
AN 167	IC-SC	Determination of Trace Concentrations of Oxyhalides and Bromide in Municipal and Bottled Waters Using a Hydroxide-Selective Column with a Reagent-Free Ion Chromatography System
AN 168	IC-UV	Determination of Trace Concentrations of Disinfection By-Product Anions and Bromide in Drinking Water Using Reagent-Free Ion Chromatography Followed by Postcolumn Addition of Iol-Dianisidine for Trace Bromate Analysis
AN 169	IC-SC	Rapid Determination of Phosphate and Citrate in Carbonated Soft Drinks Using a Reagent-Free Ion Chromatography System
AN 172	IC-SC	Determination of Azide in Aqueous Samples by Ion Chromatography with Suppressed Conductivity Detection
AN 173	IC-PAD	Direct Determination of Cyanide in Drinking Water by Ion Chromatography with Pulsed Amperometric Detection (PAD)
AN 178	IC-SC	Improved Determination of Trace Concentrations of Perchlorate in Drinking Water Using Preconcentration with Two-Dimensional Ion Chromatography and Suppressed Conductivity Detection
AN 182	IC-SC and IC-PAD	Determination of Biogenic Amines in Alcoholic Beverages by Ion Chromatography with Suppressed Conductivity and Integrated Pulsed Amperometric Detections
AN 183	IC-SC and IC-PAD	Determination of Biogenic Amines in Fermented and Non-Fermented Foods Using Ion Chromatography with Suppressed Conductivity and Integrated Pulsed Amperometric Detections
AN 187	IC-SC	Determination of sub-µg/L Bromate in Municipal Waters Using Preconcentration with Two-Dimensional Ion Chromatography and Suppressed Conductivity Detection
AN1 88	IC-PAD	Determination of Glycols and Alcohols in Fermentation Broths Using Ion-Exclusion Chromatography and Pulsed Amperometric Detection
AN 197	IC-PAD	Determination of Glucosamine in Dietary Supplements Using HPAE-PAD
AN 227	ICE-PAD	Determination of Total Cyanide in Municipal Wastewater and Drinking Water Using Ion-Exclusion Chromatography with Pulsed Amperometric Detection (ICE-PAD)
AN 248	IC-PAD	Determination of Lactose in Lactose-Free Milk Products by High-Performance Anion-Exchange Chromatography with Pulsed Amperometric Detection
AN 253	IC-PAD	HPAE-PAD Determination of Infant Formula Sialic Acids
AN 270	IC-PAD	Determination of Hydroxymethylfurfural in Honey and Biomass
AN 273	IC-SC	Determination of Organic Acids in Fruit Juices and Wines by High-Pressure IC
AN 279	IC-SC	Time Savings and Improved Reproducibility of Nitrate and Nitrite Ion Chromatography Determination in Milk Samples
AN 280	IC-PAD	Carbohydrates in Coffee: AOAC Method 995.13 vs a New Fast Ion Chromatography Method
AN 295	IC-SC	Determination of Phytic Acid in Soybeans and Black Sesame Seeds
AN 1007	IC-SC	Determination of Mono-, Di-, and Triphosphates and Citrate in Shrimp by Ion Chromatography

Thermo SCIENTIFIC

Technical Collateral: Ion Chromatography Methods

Product Number	Technique	Title
AN 1044	IC-SC	Determination of Anions in Dried Distillers Grains with Solubles
AN 1068	IC-SC	Determination of Organic Acids in Fruit Juices and Wines by High-Pressure IC
AU 132	IC-UV	Determination of Nitrite and Nitrate in drinking Water by Ion Chromatography with Direct UV Detection
AU 144	IC-UV	Determination of Hexavalent Chromium in Drinking Water Using Ion Chromatography
AU 148	IC-SC	Determination of Perchlorate in Drinking Water Using Reagent-Free Ion Chromatography
AU 150	IC-PAD	Determination of Plant-Derived Neutral Oligo- and Polysaccharides Using the CarboPac PA200
AU 151	IC-PAD	Determination of Sucralose in Reduced- Carbohydrate Colas using High-Performance Anion-Exchange Chromatography with Pulsed Amperometric Detection
AU 189	IC-SC	Determination of Choline in Infant Formula and Other Food Samples by IC
LPN 2982	IC-SC	Determination of Inorganic Anions and Organic Acids in Beverages Using a Capillary IC on a Monolith Anion-Exchange Column
PN 70743	IC-SC	Determination of Perchlorate Levels in Food and Soil Samples Using Accelerated Solvent Extraction and Ion Chromatography
TN 20	IC-PAD	Analysis of Carbohydrates by High-Performance Anion-Exchange Chromatography with Pulsed Amperometric Detection (HPAE-PAD)
TN 126	IC-SC	Determination of Organic Acids in Beer Samples Using a High-Pressure Ion Chromatography System
TN 135	IC-PAD	Determinations of Monosaccharides and Disaccharides in Beverages by Capillary HPAE-PAD

References

Sample Preparation References

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Accelerated, microwave-assisted, and conventional solvent extraction methods affect anthocyanin composition from colored grains	Abdel-Aal el-SM; Akhtar, H.; Rabalski, I.; Bryan, M.	*J. Food Sci. 79 (2),* C138–46	2014 Feb
Multiresidue method for the analysis of pesticide residues in fruits and vegetables by accelerated solvent extraction and capillary gas chromatography	Adou, K.; Bontoyan, W. R.; Sweeney, P. J.	*J. Agric. Food Chem. 49 (9),* 4153–4160	2001 Sep
The development of an optimized sample preparation for trace level detection of 17α-ethinylestradiol and estrone in whole fish tissue	Al-Ansari, A. M.; Saleem, A.; Kimpe, L. E.; Trudeau, V. L.; Blais, J. M.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 879 (30),* 3649–52	2011 Nov
Determination of polyphenolic profiles of basque cider apple varieties using accelerated solvent extraction	Alonso-Salces, R. M.; Korta, E.; Barranco, A.; Berrueta, L.A.; Gallo, B.; Vicent, F.	*J. Agric. Food Chem. 49 (8),* 3761–376	2001
Pressurized liquid extraction for the determination of polyphenols in apple	Alonso-Salces, R. M.; Korta, E.; Barranco, A.; Berrueta, L. A.; Gallo, B.; Vicente, F.;	*J. Chromatogr., A. 933 (1–2),* 37–43	2001 Nov
Methods for extraction and determination of phenolic acids in medicinal plants: a review	Arceusz, A.; Wesolowski, M.; Konieczynski, P.	*Nat. Prod. Commun. 8 (12),* 1821–9	2013 Dec
Study of an accelerated solvent extraction procedure for the determination of acaricide residues in honey by high-performance liquid chromatography-diode array detector	Bakkali, A.; Korta, E.; Berrueta, L. A.	*J. Food Protection 65 (1),* 161–166	2002
Pressurized liquid extraction of medicinal plants	Benthin, B.; Danz, H.; Hamburger, M.	*J. Chromatogr., A. 837 (1-2),* 211–9	1999 Apr
Comparison of the chemical composition of extracts from *Scutellaria lateriflora* using accelerated solvent extraction and supercritical fluid extraction versus standard hot water or 70% ethanol extraction	Bergeron, C.; Gafner, S.; Clausen, E.; Carrier, D. J.	*J. Agric. Food Chem. 53 (8),* 3076–80	2005 Apr
Polybrominated diphenyl ethers (PBDEs) in Mediterranean mussels (*Mytilus galloprovincialis*) from selected Apulia coastal sites evaluated by GC-HRMS	Bianco, G.; Novario, G.; Anzilotta, G.; Palma, A.; Mangone, A.; Cataldi, T. R.	*J. Mass Spectrom. 45 (9),* 1046–55	2010 Sep
Free and bound phenolic compounds in barley (*Hordeum vulgare* L.) flours. evaluation of the extraction capability of different solvent mixtures and pressurized liquid methods by micellar electrokinetic chromatography and spectrophotometry	Bonoli, M.; Marconi, E.; Caboni, M. F.	*J. Chromatogr., A.19; 1057 (1-2),* 1–12	2004 Nov
Pressurized liquid extraction of lipids for the determination of oxysterols in egg-containing food	Boselli, E.; Velazco, V.; Caboni, M. F.; Lercker, G.	*J. Chromatogr., A. 11; 917 (1-2),* 239–44	2001 May
Optimisation of accelerated solvent extraction of cocaine and benzoylecgonine from coca leaves	Brachet, A.; Rudaz, S.; Mateus, L.; Christen, P.; Veuthey, J-L.	*J. Sep. Sci. 24 (10-11),* 865–873	2001 Nov

Thermo SCIENTIFIC

Table of Contents

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Multi-residue determination of 130 multiclass pesticides in fruits and vegetables by gas chromatography coupled to triple quadrupole tandem mass spectrometry	Cervera, M.I.; Medina, C.; Portolés, T.; Pitarch, E; Beltrán, J.; Serrahima, E.; Pineda, L.; Muñoz, G.; Centrich, F.; Hernández, F.	*Anal. Bioanal. Chem. 397 (7),* 2873–91	2010 Aug
Influence of extraction methodologies on the analysis of five major volatile aromatic compounds of citronella grass (*Cymbopogon nardus*) and lemongrass (*Cymbopogon citratus*) grown in Thailand	Chanthai, S.; Prachakoll, S.; Ruangviriyachai, C.; Luthria, D. L.	*J. AOAC Int. 95 (3),* 763–72	2012 May-Jun
Accelerated solvent extraction of vitamin K_1 in medical foods in conjunction with matrix solid-phase dispersion	Chase, G. W.; Thompson, B.	*J. AOAC Int. 83 (2),* 407–10	2000
Development of a liquid chromatography-tandem mass spectrometry with pressurized liquid extraction method for the determination of benzimidazole residues in edible tissues	Chen, D.; Tao, Y.; Zhang, H.; Pan, Y.; Liu, Z.; Huang, L.; Wang, Y.; Peng, D.; Wang, X.; Dai, M; Yuan, Z.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 879 (19),* 1659–67	2011 Jun
Determination of 88 pesticide residues in tea using gas chromatography-tandem mass spectrometry	Chen, H.; Liu, X.; Wang, Q.; Jiang, Y.	*Se Pu. 29 (5),* 409–16	2011 May
Optimization of accelerated solvent extraction for the determination of chlorinated pesticides from animal feed	Chen, S.; Gfrerer, M.; Lankmayr, E.; Quan, X.; Yang, F.	*Chromatographia 58,* 631–636	2003
Uptake of oxytetracycline, sulfamethoxazole and ketoconazole from fertilised soils by plants	Chitescu, C. L.; Nicolau, A. I.; Stolker, A. A.	*Food Addit. Contam. Part A Chem. Anal. Control Expo. Risk Assess. 30 (6),* 1138–46	2013
Ultrasonic or accelerated solvent extraction followed by U-HPLC-high mass accuracy MS for screening of pharmaceuticals and fungicides in soil and plant samples	Chitescu, C. L.; Oosterink, E.; de Jong, J.; Stolker, A. A.	*Talanta 2012; 88,* 653–62	2011 Jan
Evaluation of analytical methods for determining pesticides in baby foods and adult duplicate-diet samples	Chuang, J. C.; Hart, K.; Chang, J. S.; Boman, L. E.; Van Emon, J. M.; Reed, A. W.	*Anal. Chim. Acta. 444 (1),* 87–95	2001 Oct
Comparison of extraction techniques and modeling of accelerated solvent extraction for the authentication of natural vanilla flavors	Cicchetti, E.; Chaintreau, A..	*J. Sep. Sci. 32 (11),* 1957–64	2009 Jun
Development of a fast and convenient method for the isolation of triterpene saponins from *Actaea racemosa* by high-speed countercurrent chromatography coupled with evaporative light scattering detection	Cicek, S. S.; Schwaiger, S.; Ellmerer, E. P.; Stuppner, H.	*Planta. Med. 76 (5),* 467–73	2010 Mar
Extraction of bitter acids from hops and hop products using pressurized solvent extraction (PSE)	Culík, J;. Jurková, M.; Horák, T.; Cejka, P; Kellner, V.; Dvorák, J.; Karásek, P.; Roth, M.	*J. Inst. Brew. 115 (3),* 220–225	2009
Comparison of methods for extraction of flavanones and xanthones from the root bark of the osage orange tree using liquid chromatography	da Costa, C. T.; Margolis, S. A.; Benner, Jr. B.A.; Horton, D.	*J. Chromatogr., A. 831 (2),* 167–178	1999 Jan
Pressurized liquid extraction prior to liquid chromatography with electrochemical detection for the analysis of vitamin E isomers in seeds and nuts	Delgado-Zamarreño, M. M.; Bustamante-Rangel, M.; Sánchez-Pérez, A.; Carabias-Martínez, R.	*J. Chromatogr., A. 12; 1056 (1-2),* 249–52	2004 Nov

Thermo SCIENTIFIC

Table of Contents

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Pressurized fluid extraction of carotenoids from *Haematococcus pluvialis* and *Dunaliella salina* and kavalactones from *Piper methysticum*	Denery, J. R.; Dragull, K.:Tang, C. S.; Li, Q. X.	*Anal. Chim. Acta. 501 (2),* 175–181	2004 Jan
Development and comparison of two multiresidue methods for the analysis of 17 mycotoxins in cereals by liquid chromatography electrospray ionization tandem mass spectrometry	Desmarchelier, A.; Oberson, J. M.; Tella, P.; Gremaud, E.; Seefelder, W.; Mottier, P.	*J. Agric. Food Chem. 58 (13),* 7510–9	2010 Jul
Identification, extraction and quantification of the synthetic cannabinoid JWH-018 from commercially available herbal marijuana alternatives	Dunham, S. J.; Hooker, P. D.; Hyde, R. M.	*Forensic Sci. Int. 223 (1-3),* 241–4	2012 Nov
Evaluation of polyphenol contents in differently processed apricots using accelerated solvent extraction followed by high-performance liquid chromatography-diode array detector	Erdogan, S.; Erdemoglu, S.	*Int. J. Food Sci. Nutr. 62 (7),* 729–39	2011 Nov
Determination of 2,4,6-trichloroanisole and guaiacol in cork stoppers by pressurised fluid extraction and gas chromatography–mass spectrometry	Ezquerro, Ó.; Garrido-López, Á.; Tena, M. T.	*J. Chromatogr., A. 1102 (12),* 18–24	2006 Jan
Multiwalled carbon nanotubes as matrix solid-phase dispersion extraction absorbents to determine 31 pesticides in agriculture samples by gas chromatography-mass spectrometry	Fang, G.; Min, G.; He, J.; Zhang, C.; Qian, K.; Wang, S.	*J. Agric. Food Chem. 57 (8),* 3040–5	2009 Apr
High-anthocyanin strawberries through cultivar selection	Fredericks, C. H.; Fanning, K. J.; Gidley, M. J.; Netzel, G.; Zabaras, D.; Herrington, M.; Netzel, M.	*J. Sci. Food Agric. 93 (4),* 846–52	2013 Mar
Optimal extraction and fingerprint analysis of *Cnidii fructus* by accelerated solvent extraction and high performance liquid chromatographic analysis with photodiode array and mass spectrometry detections	Gao, F.; Hu, Y.; Ye, X.; Li, J.; Chen, Z.; Fan, G.	*Food Chem. 1 141 (3),* 1962–71	2013 Dec
Simultaneous analysis of seven alkaloids in *Coptis-evodia* herb couple and Zuojin pill by UPLC with accelerated solvent extraction	Gao, X.; Yang, X. W.; Marriott, P. J.	*J. Sep. Sci. 33 (17-18),* 2714–22	2010 Sep
Determination of chromones in *Dysophylla stellata* by HPLC: method development, validation and comparison of different extraction methods	Gautam, R.; Srivastava, A.; Jachak, S. M.	*Nat. Prod. Commun. 5 (4),* 555–8	2010 Apr
Comparison of different extraction techniques for the determination of chlorinated pesticides in animal feed	Gfrerer, M.; Chen, S.; Lankmayr, E.; Xie, Q.; Yang, F.	*Anal. Bioanal. Chem. 378 (7),* 1861–1867	2004
Speciation analysis of selenium compounds in yeasts using pressurised liquid extraction and liquid chromatography–microwave-assisted digestion–hydride generation–atomic fluorescence spectrometry	Gómez-Ariza, J. L.; Caro de la Torre, M. A.; Giráldez, I.; Morales, E.	*Anal. Chim. Acta. 524, (1–2),* 305–314	2004 Oct

Thermo SCIENTIFIC

Table of Contents

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Multianalysis of 35 mycotoxins in traditional Chinese medicines by ultra-high-performance liquid chromatography-tandem mass spectrometry coupled with accelerated solvent extraction	Han, Z.; Ren Y.; Zhu, J.; Cai, Z.; Chen, Y.; Luan, L.; Wu, Y.	*J. Agric. Food Chem. 60 (33),* 8233-47.	2012 Aug
Pressurized liquid extraction-capillary electrophoresis-mass spectrometry for the analysis of polar antioxidants in rosemary extracts	Herrero, M.; Arráez-Román, D.; Segura A.; Kenndler, E.; Gius, B.; Raggid, M. A.; Ibáñez, E.; Cifuentes, A.	*J. Chromatogr., A.1084 (1-2),* 54–62.	2005 Aug
Accelerated solvent extraction of alkylresorcinols in food products containing uncooked and cooked wheat	Holt, M D.; Moreau, R A,.;DerMarderosian, A.; McKeown, N.; Jacques, P. F.	*J. Agric. Food Chem. 60 (19),* 4799–802	2012 May
Application of response surface methodology to optimize pressurized liquid extraction of antioxidant compounds from sage (*Salvia officinalis* L.), basil (*Ocimum basilicum* L.) and thyme (*Thymus vulgaris* L.)	Hossain, M. B.; Brunton, N. P.; Martin-Diana, A. B.; Barry-Ryan, C.	*Food Funct. 1(3),* 269–77	2010 Dec
A review of modern sample-preparation techniques for the extraction and analysis of medicinal plants	Huie, C. W.	*Anal. Bioanal. Chem. 373 (1-2),* 23–30.	2002 May
Polychlorinated dioxins, furans, and biphenyls, and polybrominated diphenyl ethers in a U.S. meat market basket and estimates of dietary intake	Huwe, J. K.; Larsen, G. L.	*Environ. Sci. Technol. 39 (15),* 5606–5611	2005
Study of the effect of sample preparation and cooking on the selenium speciation of selenized potatoes by HPLC with ICP-MS and electrospray ionization MS/MS	Infante, H. G.; Borrego, A. A.; Peachey, E.; Hearn, R.; O'Connor, G.; Barrera, T G.; Ariza, J. L.	*J. Agric. Food Chem. 57(1),* 38–45.	2009 Jan
Pentacyclic triterpene distribution in various plants – rich sources for a new group of multi-potent plant extracts	Jäger, S.; Trojan, H.; Kopp, T.; Laszczyk, M. N.; Scheffler, A.	*Molecules. 14 (6),* 2016–31.	2009 Jun
Comprehensive multiresidue method for the simultaneous determination of 74 pesticides and metabolites in traditional Chinese herbal medicines by accelerated solvent extraction with high-performance liquid chromatography/tandem mass spectrometry	Jia, Z.; Mao, X.; Chen, K.; Wang, K.; Ji S.	*J. AOAC Int.; 93(5),* 1570–88.	2010 Sep-Oct
Gas chromatography-mass spectrometry (GC-MS) method for the determination of 16 European priority polycyclic aromatic hydrocarbons in smoked meat products and edible oils	Jira, W.; Ziegenhals, K.; Speer, K.	*Food Addit. Contam. Part A Chem. Anal. Control Expo. Risk Assess. 25 (6),* 704–13.	2008 Jun
Assessing pressurized liquid extraction for the high-throughput extraction of marine-sponge-derived natural products	Johnson, T. A.; Morgan, M. V.; Aratow, N. A.; Estee, S. A.; Sashidhara, K. V.; Loveridge, S. T.; Segraves, N L.; Crews, P.	*J. Nat. Prod. 73 (3),* 359–64.	2010 Mar
Lipophilic stinging nettle extracts possess potent anti-inflammatory activity, are not cytotoxic and may be superior to traditional tinctures for treating inflammatory disorders	Johnson, T. A.; Sohn, J.; Inman, W. D.; Bjeldanes, L. F.; Rayburn, K.	*Phytomedicine 20(2),* 143–7.	2013 Jan
Effects of solvent and temperature on pressurized liquid extraction of anthocyanins and total phenolics from dried red grape skin	Ju Z. Y.; Howard, L. R.	*J. Agric. Food Chem. 51 (18),* 5207–13.	2003 Aug

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Accelerated solvent extraction of ochratoxin A from rice samples	Juan, C.; González, L.; Soriano, J. M.; Moltó, J. C.; Mañes, J.	*J. Agric. Food Chem. 53 (24),* 9348–9351	2005
Accelerated solvent extraction of paclitaxel and related compounds from the bark of *Taxus cuspidate*	Kawamura, F.; Kikuchi, Y.; Ohira, T.; Yatagai, M.	*J. Nat. Prod. 62 (2),* 244–7.	1999 Feb
Determination of polybromodiphenyl ethers (PBDEs) in milk cream by gas chromatography-mass spectrometry	Kinani, S.; Bouchonnet, S.; Abjean, J.; Campargue, C.	*Food Addit. Contam. Part A Chem. Anal. Control Expo. Risk Assess. 25 (8),* 1007–14	2008 Aug
Determination of isoflavones in soy bits by fast column high-performance liquid chromatography coupled with UV–visible diode-array detection	Klejdus, B.; Mikelová, R.; Petrlová, J.; Potešil, D.; Adam, V.; Stiborová, J.; Hodek, P.; Vacek, J.; Kizek, R.; Kubán, V.	*J. Chromatogr., A. 1084 (1–2), 19,* 71–79	2005 Aug
Accelerated solvent extraction of lignin from *Aleurites moluccana* (candlenut) nutshells	Klein, A. P.; Beach, E. S.; Emerson, J. W.; Zimmerman, J. B.	*J. Agric. Food Chem. 58 (18),* 10045–8	2010 Sep
Application of TLC method with video scanning in estimation of daily dietary intake of specific flavonoids – preliminary studies	Koch, W.; Kukuła-Koch, W.; Marzec, Z.; Marc, D.	*Acta Pol. Pharm. 70 (4),* 611–20	2013 Jul-Aug
Evaluation of a fibrous cellulose drying agent in supercritical fluid extraction and pressurized liquid extraction of diverse pesticides	Lehotay, S. J.; Lee, C. H.	*J. Chromatogr., A.785 (1-2),* 313–27	1997 Oct
Application of accelerated solvent extraction to the investigation of saikosaponins from the roots of *Bupleurum falcatum*	Li, W.; Liu, Z.; Wang, Z.; Chen, L.; Sun, Y.; Hou, J.; Zheng, Y.	*J. Sep. Sci. 33 (12),* 1870–6	2010 Jun
Applicability of accelerated solvent extraction for synthetic colorants analysis in meat products with ultrahigh performance liquid chromatography-photodiode array detection	Liao, Q. G.; Li ,W. H.; Luo, LG.	*Anal. Chim. Acta. 716,* 128–32	2012 Feb
Extraction, isolation, and purification of analytes from samples of marine origin – a multivariate task	Liguori, L.; Bjørsvik, H. R.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 910,* 46–53	2012 Dec
Investigation on levels of polybrominated diphenyl ethers in retail fish and egg products in Shenzhen	Liu, B.; Zhang, L. S.; Zhang, J. Q.; Jiang, Y. S.; Zhou, J.; Huang, H. Y.	*Zhonghua Yu Fang Yi Xue Za Zhi. 45 (12),* 1068–72	2011 Dec
Characterization of secondary volatile profiles in *Nigella sativa* seeds from two different origins using accelerated solvent extraction and gas chromatography-mass spectrometry	Liu, X.; Abd El-Aty, A. M.; Cho, S. K.; Yang, A.; Park, J. H.; Shim, J. H.	*Biomed. Chromatogr. 26 (10),* 1157–62	2012 Oct
Accelerated solvent extraction of monacolin K from red yeast rice and purification by high-speed counter-current chromatography	Liu, Y.; Guo, X.; Duan, W.; Wang, X.; Du, J.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 878 (28),* 2881–5	2010 Oct
Multiresidue determination of organophosphorus pesticides in ginkgo leaves by accelerated solvent extraction and gas chromatography with flame photometric detection	Lu, Y.; Yi, X.	*J. AOAC Int. 88 (3),* 729–735	2005

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Influence of sample preparation on assay of phenolic acids from eggplant	Luthria, DL.; Mukhopadhyay, S.	*J. Agric. Food Chem. 54 (1),* 41–47	2006
Pressurised solvent extraction for organotin speciation in vegetable matrices	Marcic, C.; Lespe,s G.; Potin-Gautier, M.	*Anal. Bioanal. Chem. 382 (7),* 1574–83	2005 Aug
Comparison of different methods for the determination of the oil content in oilseeds	Matthäus, B.; Brühl, L.	*J. AOCS 78* 95–102.	2001 Jan
A comparison of automated and traditional methods for the extraction of arsenicals from fish	McKiernan, J. W.; Creed, J. T.; Brockhoff, C. A.; Caruso, J. A.; Lorenzana, R. M.	*J. Anal. At. Spectrom. 14,* 607–613	1999
Subcritical solvent extraction of anthocyanins from dried red grape pomace	Monrad, J. K.; Howard, L. R.; King, J.;, Srinivas, K.; Mauromoustakos, A.	*J. Agric. Food Chem. 58 (5),* 2862–8	2010 Mar
Subcritical solvent extraction of procyanidins from dried red grape pomace	Monrad, J. K.; Howard, L. R.; King, J. W.; Srinivas, K.; Mauromoustakos, A.	*J. Agric. Food Chem.58 (7),* 4014–21	2010 Apr
Pressurized liquid extraction of polar and nonpolar lipids in corn and oats with hexane, methylene chloride, isopropanol, and ethanol	Moreau, R. A.; Powell, M. J.; Singh, V.	*J. Oil Fat Industr. 80 (11),* 1063–1067	2003 Jan
Accelerated solvent extraction for natural products isolation	Mottaleb, M. A.; Sarker, S. D.	*Methods Mol. Biol. 864,* 75–87	2012
Optimization of extraction process for phenolic acids from black cohosh (*Cimicifuga racemosa*) by pressurized liquid extraction	Mukhopadhyay, S,.;Luthria, D. L,.;Robbins, R. J.	*J. Sci. Food Agric. 86 (1),* 156–162, 15	2006 Jan
Anxiolytic activity of a supercritical carbon dioxide extract of *Souroubea sympetala* (Marcgraviaceae)	Mullally, M.; Kramp, K.; Cayer, C.; Saleem, A.; Ahmed, F, McRae, C.; Baker, J.; Goulah, A.; Otorola, M.; Sanchez, P.; Garcia, M.; Poveda, L.; Merali, Z.; Durst, T.; Trudeau, V. L.; Arnason, J. T.	*Phytother. Res. 25 (2),* 264–70	2011 Feb
On-line clean-up of pressurized liquid extracts for the determination of polychlorinated biphenyls in feedingstuffs and food matrices using gas chromatography–mass spectrometry	Müller, A.; Björklund, E.; von Holst, C.	*J. Chromatogr., A. 925 (1–2),* 197–205	2001 Aug
Analysis of multiple herbicides in soybeans using pressurized liquid extraction and capillary electrophoresis	Nemoto, S.; Lehotay, S. J.	*J. Agric. Food Chem.; 46 (6),* 2190–2199	1998
Comparison of sample preparation methods, validation of an UPLC-MS/MS procedure for the quantification of tetrodotoxin present in marine gastropods and analysis of pufferfish	Nzoughet, J. K.; Campbell, K.; Barnes, P.; Cooper, K. M.; Chevallier, O. P, Elliott, C. T.	*Food Chem. 15; 136 (3-4),* 1584–9	2013 Feb
Multiresidue analysis of pesticides in vegetables and fruits using two-layered column with graphitized carbon and water absorbent polymer	Obana, H.; Akutsu, K.; Okihashi, M.; Hori, S.	*The Analyst 123,* 711–714	1998
Analysis of 2-alkylcyclobutanones with accelerated solvent extraction to detect irradiated meat and fish	Obana, H.; Furuta, M.; Tanaka, Y.	*J. Agric. Food Chem. 53 (17),* 6603–8	2005 Aug

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Determination of organophosphorus pesticides in foods using an accelerated solvent extraction system	Obana, H.; Kikuchi, K.; Okihashi, M.; Hori, S.	*Analyst 122 (3),* 217–20	1997 Mar
Pressurized hot water extraction of berberine, baicalein and glycyrrhizin in medicinal plants	Ong, E. S.; Shea Mei, L.	*Anal. Chim. Acta. 482 (1),* 81–89	2003 Apr
Pressurized liquid extraction of berberine and aristolochic acids in medicinal plants	Ong E. S.; Woo S. O.; Yong, Y. K.	*J. Chromatogr., A. 904 (1),* 57–6422	2000 Dec
Rapid determination of pesticide multiresidues in vegetables and fruits by accelerated solvent extraction coupled with online gel permeation chromatography-gas chromatography-mass spectrometry	Ouyang, Y.; Tang, H.; Wu, Y.; Li, G.	*Se Pu. 30(7),* 654–9	2012 Jul
Determination of zearalenone from wheat and corn by pressurized liquid extraction and liquid chromatography-electrospray mass spectrometry	Pallaroni, L.; von Holst, C.	*J. Chromatogr., A. 993,* 39–45	2003
Development of an extraction method for the determination of zearalenone in corn using less organic solvents	Pallaroni, L.; von Holst, C.	*J. Chromatogr., A. 5 1055 (1-2),* 247–9	2004 Nov
Stability of phenolic compounds during extraction with superheated solvents	Palma, M.; Piñeiro, Z.; Barroso, C. G.	*J. Chromatogr., A. 6 921 (2),* 169–74	2001 Jul
Extraction and analysis of trace amounts of cyclonite (RDX) and its nitroso-metabolites in animal liver tissue using gas chromatography with electron capture detection (GC-ECD)	Pan, X.; Zhang, B.; Cobb, G. P.	*Talanta 67 (4),* 816–23	2005 Oct
Simultaneous determination of 405 pesticide residues in grain by accelerated solvent extraction then gas chromatography-mass spectrometry or liquid chromatography-tandem mass spectrometry	Pang, G.; Liu, Y.; Fan, C.; Zhang, J.; Cao, Y.; Li, X.; Li, Z.; Wu, Y.; Guo, T.	*Anal. Bioanal. Chem. 384,* 1366–1408	2006 Mar
Automated sample preparation by pressurized liquid extraction-solid-phase extraction for the liquid chromatographic-mass spectrometric investigation of polyphenols in the brewing process	Papagiannopoulos, M.; Mellenthin, A.	*J. Chromatogr., A. 8 976 (1-2),* 345–8	2002 Nov
Online coupling of pressurized liquid extraction, solid-phase extraction and high-performance liquid chromatography for automated analysis of proanthocyanidins in malt	Papagiannopoulos, M.; Zimmermann, B.; Mellenthin, A.; Krappe, M.; Maio, G.; Galensa, R.	*J. Chromatogr., A. 7 958 (1-2),* 9–16	2002 Jun
Simultaneous determination of 13 quinolones from feeds using accelerated solvent extraction and liquid chromatography	Pecorelli, I.; Galarini, R.; Bibi, R.; Floridi, A. I.; Casciarri, E.; Floridi, A.	*Anal. Chim. Acta. 483 (1-2),* 81–89	2003 April
Comparison of soxhlet, ultrasound-assisted and pressurized liquid extraction of terpenes, fatty acids and Vitamin E from *Piper gaudichaudianum* Kunth	Péres, V. F.; Saffi, J.; Melecchi, M. I.; Abad, F. C.; de Assis Jacques, R.; Martinez, M. M.; Oliveira, E. C.; Caramão, E. B.	*J. Chromatogr., A. 1105 (1-2),* 115–8	2006 Feb
Pressurised fluid extraction (PFE) as an alternative general method for the determination of pesticide residues in rape seed	Pihlström, T.; Isaac, G.; Waldebäck, M.; Osterdahl, B. G.; Markides, K. E.	*Analyst 127 (4),* 554–9	2002 Apr
Determination of catechins by means of extraction with pressurized liquids	Piñeiro, Z.; Palma, M.; Barroso C. G.	*J. Chromatogr., A. 13 1026 (1-2),* 19–23.	2004 Feb

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
An improved clean-up strategy for simultaneous analysis of polychlorinated diben-zo-p-dioxins (PCDD), polychlorinated dibenzofurans (PCDF), and polychlorinated biphenyls (PCB) in fatty food samples	Pirard, C.; Focant, J. F.; De, P. E.	*Anal. Bioanal. Chem. 372 (2),* 373–81.	2002 Jan
Extraction of polar and hydrophobic pollutants using accelerated solvent extraction (ASE)	Pörschmann, J., Plugge, J.	*Fresen. J. Anal. Chem. 364 (7),* 643–645	1999
Quantification of the total amount of artemisinin in leaf samples by thin layer chromatography	Quennoz, M.; Bastian, C.; Simonnet, X.; Grogg, A. F.	*Chimia (Aarau) 64 (10),* 755–7.	2010
Determination of fat in dairy products using pressurized solvent extraction	Richardson, R. K.	*J. AOAC Int. 84 (5),* 1522–1533	2001
Influence of altitudinal variation on the content of phenolic compounds in wild populations of *Calluna vulgaris,* Sambucus nigra, and *Vaccinium myrtillus*	Rieger, G.; Müller, M.; Guttenberger, H.; Bucar, F.	*J. Agric. Food Chem. 56 (19),* 9080–6.	2008 Oct
Pressurized liquid extraction of isoflavones from soybeans	Rostagno, M. A.; Palma, M.; Barroso, C. G.	*Anal. Chim. Acta. 522 (2),* 169–177.	2004 Sep
A multi-residue method for the analysis of organophosphorus residues in cooked and polished rice using accelerated solvent extraction and dispersive-solid phase extraction (D-SPE) technique and uncertainty measurement	Sanyal, D.; Rani, A.; Alam, S.	*J. Environ. Sci. Health, B 44 (7),* 706–16.	2009 Sep
Accelerated solvent extraction of lipids for determining the fatty acid composition of biological material	Schäfer, K.	*Anal. Chim. Acta. 358 (1),* 69–77	1998 Jan
HPLC analysis of kaempherol and quercetin derivatives isolated by different extraction techniques from plant matrix	Skalicka-Wozniak, K.; Szypowski, J.; Głowniak, K.	*J. AOAC Int. 94 (1),* 17–21.	Jan-Feb 2011
Statistical evaluation of fatty acid profile and cholesterol content in fish (common carp) lipids obtained by different sample preparation procedures	Spiric, A.; Trbovic, D.; Vranic, D.; Djinovic, J.; Petronijevic, R.; Matekalo-Sverak, V.	*Anal. Chim. Acta. 672 (1-2), 66–71.*	2010 Jul
Application of accelerated solvent extraction in the analysis of organic contaminants, bioactive and nutritional compounds in food and feed	Sun, H.; Ge, X.; Lv, Y.; Wang, A.	*J. Chromatogr., A. 1237,* 1–23.	2012 May
Development of an accelerated solvent extraction, ultrasonic derivatisation LC-MS/MS method for the determination of the marker residues of nitrofurans in freshwater fish	Tao, Y.; Chen, D.; Wei, H.; Yuanhu, P.; Liu, Z.; Huang, L.; Wang, Y.; Xie, S.; Yuan, Z.	*Food Addit. Contam. Part A Chem. Anal. Control Expo. Risk Assess. 29 (5),* 736–45.	2012
Simultaneous determination of lincomycin and spectinomycin residues in animal tissues by gas chromatography-nitrogen phosphorus detection and gas chroma-tography-mass spectrometry with accelerated solvent extraction	Tao, Y.; Chen, D.; Yu, G,.;Yu, H.; Pan, Y.; Wang, Y.; Huang, L.; Yuan, Z.	*Food Addit. Contam. Part A Chem. Anal. Control Expo. Risk Assess. 28 (2),* 145–54.	2011 Feb
Determination of 17 macrolide antibiotics and avermectins residues in meat with accelerated solvent extraction by liquid chromatography-tandem mass spectrometry	Tao, Y.; Yu, G.; Chen, D.; Pan, Y.; Liu, Z.; Wei, H.; Peng, D.; Huang, L.; Wang, Y.; Yuan, Z.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 897,* 64–71.	2012 May
Determination of seven toxaphene congeners in ginseng and milkvetch root by gas chromatography tandem mass spectrometry	Tian, S.; Mao, X.; Miao, S.; Jia, Z.; Wang, K.; Ji, S.	*Se Pu. 30 (1),* 14–20.	2012 Jan

Thermo SCIENTIFIC

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
A consecutive preparation method based upon accelerated solvent extraction and high-speed counter-current chromatography for isolation of aesculin from *Cortex fraxinus*	Tong, X.; Zhou, T, Xiao, X.; Li, G.	*J. Sep. Sci. 35 (24),* 3609–14	2012 Dec
Characterization of anthocyanins and anthocyanidins in purple-fleshed sweetpotatoes by HPLC-DAD/ESI-MS/MS	Truong, V. D.; Deighton, N.; Thompson, R. T.; McFeeters, R. F.; Dean, L. O.; Pecota, K. V.; Yencho, G. C.	*J. Agric. Food Chem. 58 (1),* 404–10	2010 Jan
Fat extraction from acid- and base-hydrolyzed food samples using accelerated solvent extraction	Ullah, S. M.; Murphy, B.; Dorich, B.; Richter, B.; Srinivasan, K.	*J. Agric. Food Chem. 59 (6),* 2169–74.	2011 Mar
Analysis of zearalenone in cereal and swine feed samples using an automated flow-through immunosensor	Urraca, J. L.; Benito-Peña, E.; Pérez-Conde, C.; Moreno-Bondi, M. C.; Pestka, J. J.	*J. Agric. Food Chem. 53 (9),* 3338–3344	2005
Accelerated solvent extraction and gas chromatography/mass spectrometry for determination of polycyclic aromatic hydrocarbons in smoked food samples	Wang, G.; Lee, A. S.; Lewis, M.; Kamath, B.; Archer, R. K.	*J. Agric. Food Chem. 47 (3),* 1062–6.	1999 Mar
Subcritical water extraction of alkaloids in *Sophora flavescens* Ait. and determination by capillary electrophoresis with field-amplified sample stacking	Wang, H.; Lu, Y.; Chen, J.; Li, J.; Liu, S.	*J. Pharm. Biomed .Anal. 58,* 146–51.	2012 Jan
Evaluation of Soxhlet extraction, accelerated solvent extraction and microwave-assisted extraction for the determination of polychlorinated biphenyls and polybrominated diphenyl ethers in soil and fish samples	Wang, P.; Zhang, Q.; Wang, Y.; Wang, T.; Li X.; Ding, L.; Jiang, G.	*Anal. Chim. Acta. 663 (1),* 43–8.	2010 Mar
Determination of ten pesticides of pyrazoles and pyrroles in tea by accelerated solvent extraction coupled with gas chromatography-tandem mass spectrometry	Xu, D.; Lu, S.; Chen, D.; Lan, J.; Zhang, Z.; Yang, F.; Zhou, Y.	*Se Pu.; 31 (3),* 218–22.	2013 Mar
Online cleanup of accelerated solvent extractions for determination of adenosine 5'-triphosphate (ATP), adenosine 5'-diphosphate (ADP), and adenosine 5'-monophosphate (AMP) in royal jelly using high-performance liquid chromatography	Xue, X.; Wang, F.; Zhou, J.; Chen, F.; Li, Y.; Zhao, J.	*J. Agric. Food Chem. 57 (11),* 4500–5.	2009 Jun
Identification and quantitation of eleven sesquiterpenes in three species of *Curcuma* rhizomes by pressurized liquid extraction and gas chromatography–mass spectrometry	Yang, F. Q.; Li ,S.; Chen, Y.; Lao, S. C.; Wang, YT.; Dong, T. T. X.; Tsim, K. W. K.	*J. Pharm. Biomed. Anal. 39 (3/4),* 552–558	2005 Sep
Dispersive solid-phase extraction cleanup combined with accelerated solvent extraction for the determination of carbamate pesticide residues in *Radix glycyrrhizae* samples by UPLC-MS-MS	Yang, R. Z.; Wang, J. H.; Wang, M. L.; Zhang, R.; Lu, X. Y.; Liu, W. H.	*J. Chromatogr. Sci. 49 (9),* 702–8.	2011 Oct
Simultaneous determination of amitraz and its metabolite residue in food animal tissues by gas chromatography-electron capture detector and gas chromatography-mass spectrometry with accelerated solvent extraction	Yu, H.; Tao, Y.; Le, T.; Chen, D.; Ishsan, A.; Liu, Y, Wang, Y.; Yuan, Z.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 878 (21),* 1746–52.	2010 Jul
Simultaneous determination of fluoroquinolones in foods of animal origin by a high performance liquid chromatography and a liquid chromatography tandem mass spectrometry with accelerated solvent extraction	Yu, H.; Tao, Y.; Chen, D.; Pan, Y.; Liu, Z.; Wang, Y.; Huang, L.; Dai, M.; Peng, D.; Wang, X.; Yuan, Z.	*J. Chromatogr. B Analyt. Technol. Biomed. Life Sci. 885-886,* 150–9.	2012 Feb

Thermo SCIENTIFIC

Table of Contents

Peer Reviewed Journals: Sample Preparation Methods

Title	Authors	Publication	Publication Date
Determination of pentachlorophenol residue in meat and fish by gas chromatography-electron capture detection and gas chromatography-mass spectrometry with accelerated solvent extraction	Zhao, D.	*J. Chromatogr. Sci.*	2013 May
Response surface modeling and optimization of accelerated solvent extraction of four lignans from *fructus schisandrae*	Zhao, L. C.; He, Y, Deng.; X, Yang, G. L.; Li, W.; Liang, J.; Tang, Q. L.	*Molecules. 17 (4),* 3618–29	2012 Mar
Determination of acetanilide herbicides in cereal crops using accelerated solvent extraction, solid-phase extraction and gas chromatography-electron capture detector	Zhang, Y.; Yang, J.; Shi, R.; Su, Q.; Yao, L.; Li, P.	*J. Sep. Sci. 34 (14),* 1675–82	2011 Jul
Application of accelerated solvent extraction coupled with high-performance counter-current chromatography to extraction and online isolation of chemical constituents from *Hypericum perforatum* L	Zhang, Y.; Liu, C.; Yu, M.; Zhang, Z.; Qi, Y.; Wang, J.; Wu, G.; Li, S.; Yu, J.; Hu, Y.	*J. Chromatogr., A. 1218 (20),* 2827–34	2011 May
Analysis of volatile components in Qingshanlvshui tea using solid-phase microextraction/accelerated solvent extraction-gas chromatography-mass spectrometry	Zhan, J.; Lu, S.; Meng, Z.; Xiang, N.; Cao, Q.; Miao, M.	*Se Pu. 26 (3),* 301–5.	2008 May

Thermo SCIENTIFIC

Technical Collateral: Sample Preparation Methods

Product Number	Technique	Title
AN 326	HPLC-UV	Extraction of Drugs from Animal Feeds Using Accelerated Solvent Extraction (ASE)
AN 335	HPLC-UV	Accelerated Solvent Extraction (ASE) of Active Ingredients from Natural Products
AN 356	IC-conductivity	Determination of Perchlorate in Vegetation Samples Using Accelerated Solvent Extraction and Ion Chromatography
AN 357	HPLC	Extraction of Phenolic Acids from Plant Tissue Using Accelerated Solvent Extraction (ASE)
AN 363	HPLC	Extraction of Herbal Marker Compounds Using Accelerated Solvent Extraction Compared to Traditional Pharmacopoeia Protocols

Thermo SCIENTIFIC

www.thermoscientific.com/liquidchromatography

Thermo Fisher Scientific, Sunnyvale, CA USA is ISO 9001:2008 Certified.

Africa +43 1 333 50 34 0
Australia +61 3 9757 4300
Austria +43 810 282 206
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China 800 810 5118 (free call domestic)
400 650 5118
Denmark +45 70 23 62 60
Europe-Other +43 1 333 50 34 0
Finland +358 9 3291 0200
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9494
Italy +39 02 950 591
Japan +81 45 453 9100
Korea +82 2 3420 8600
Latin America +1 561 688 8700
Middle East +43 1 333 50 34 0
Netherlands +31 76 579 55 55
New Zealand +64 9 980 6700
Norway +46 8 556 468 00
Russia/CIS +43 1 333 50 34 0
Singapore +65 6289 1190
Spain +34 914 845 965
Sweden +46 8 556 468 00
Switzerland +41 61 716 77 00
UK +44 1442 233555
USA +1 800 532 4752

Thermo SCIENTIFIC

A Thermo Fisher Scientific Brand

AI71474-EN 0215S