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Chromatography for Foods and Beverages

Contaminants Applications Notebook

Delivering the Highest Quality and Safety

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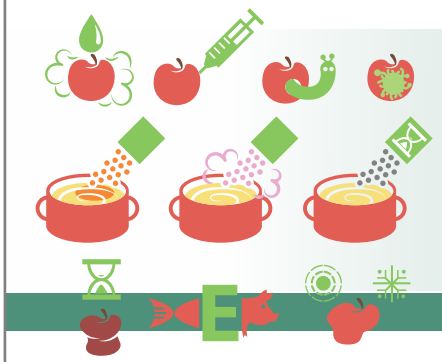

Contaminants

Introduction

Increasingly global food supply chains have raised concerns about food safety. Products are grown and processed in widely differing environments under a variety of regulatory frameworks, travel thousands of miles, are kept in various storage conditions, experience temperature fluctuations that may affect shelf life, and are handled by many different people. At any point in this process, products can be contaminated or may become unfit for consumption. Contaminants may originate from agricultural sources, such as pesticides, animal growth hormones, or antibiotics; environmental sources, such as water and air pollutants; or from food production processes, via contamination or adulteration.

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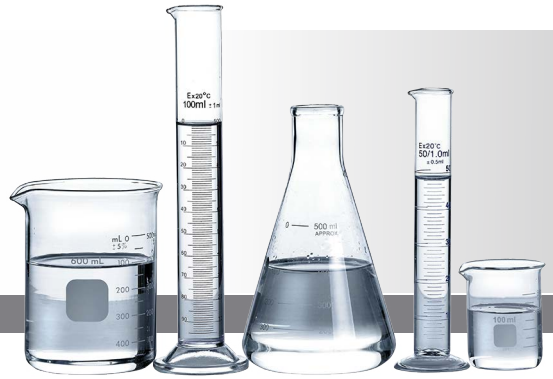

Analytical Technologies

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.

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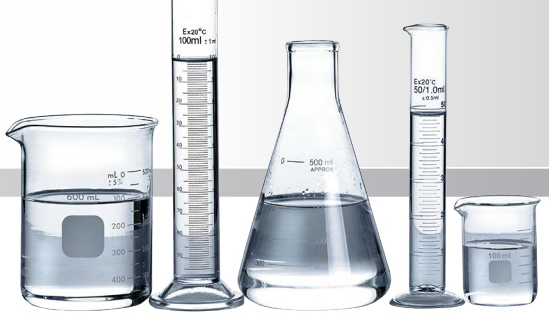


The Vanquish UHPLC System

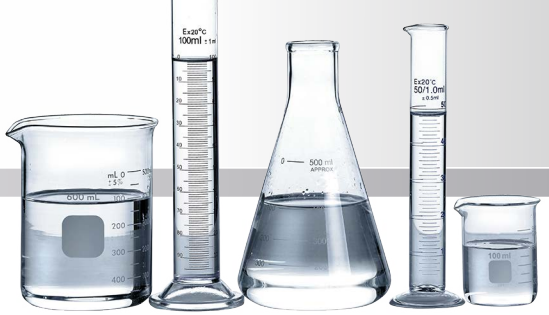
The next generation in UHPLC innovations

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.

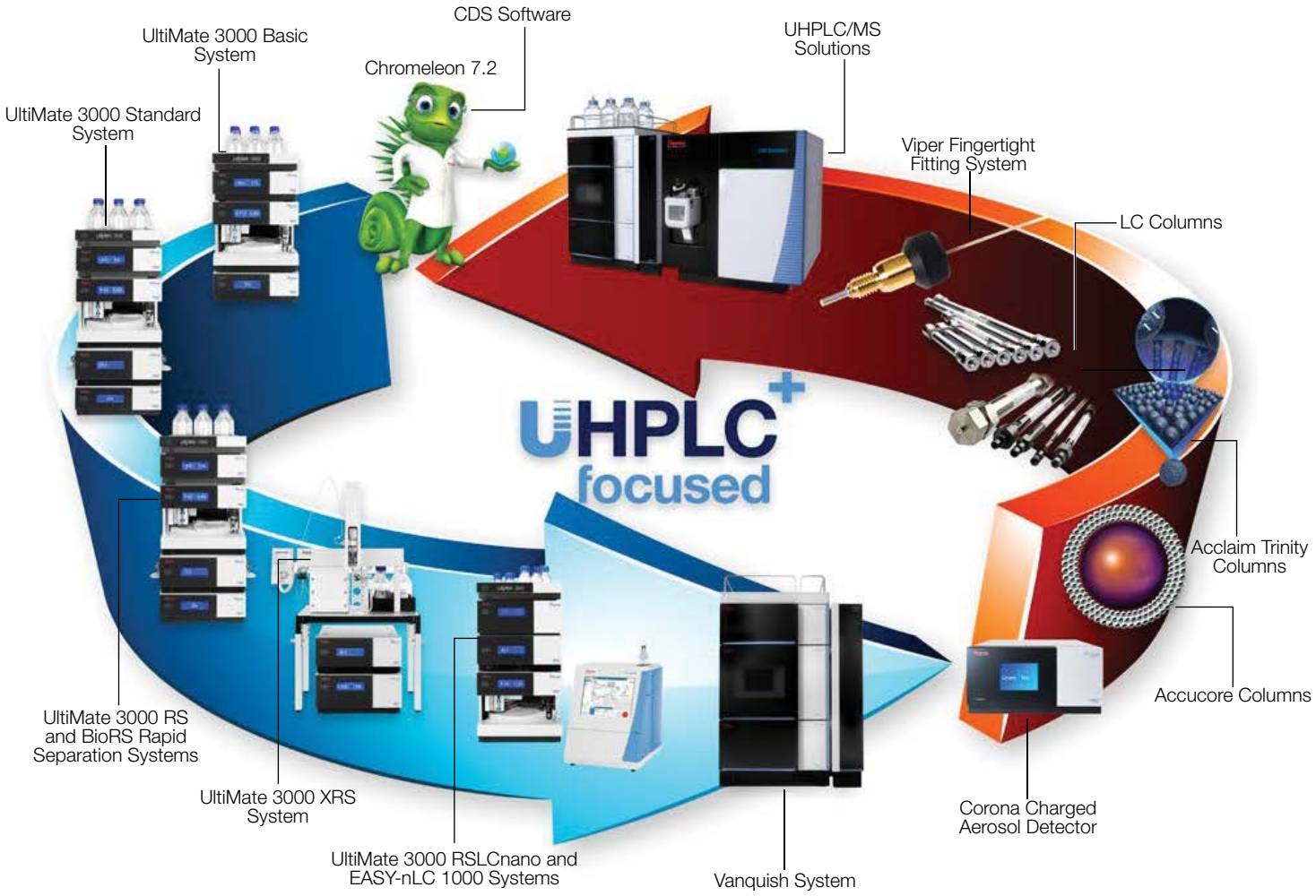
Delivering the new standard in UHPLC

- 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



UHPLC Portfolio



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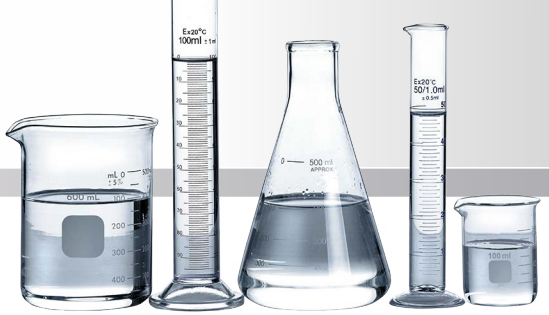


UltiMate 3000 UHPLC+ Systems

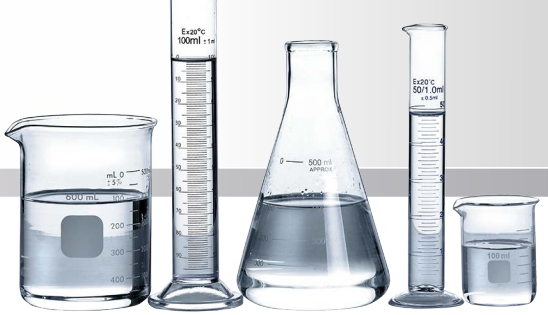
Best-in-class HPLC systems for all your chromatography needs

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



UltiMate 3000 UHPLC+ Systems

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

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.

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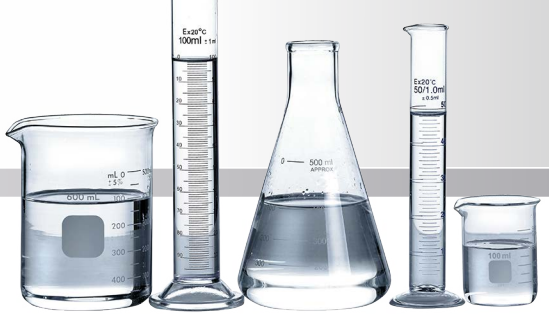


Advanced Detection Capabilities

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.

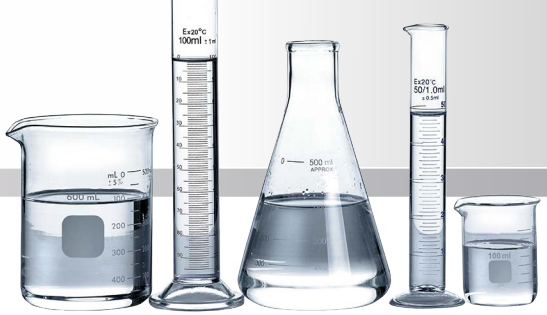
- High sensitivity – single-digit nanogram on column
- Consistent response – independent of chemical structure
- Wide dynamic range – to four orders of magnitude or greater
- Simple to use – easy to integrate with any HPLC/UHPLC system

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



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

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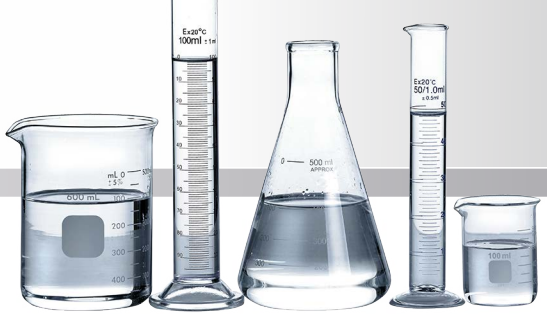


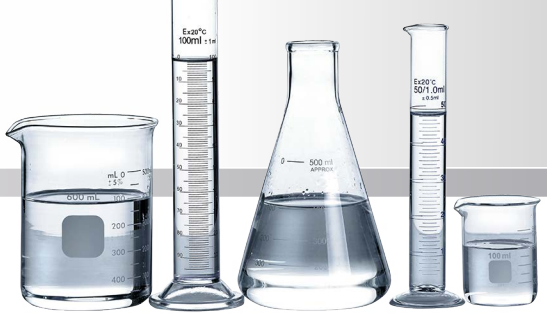
Advanced Detection Capabilities

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

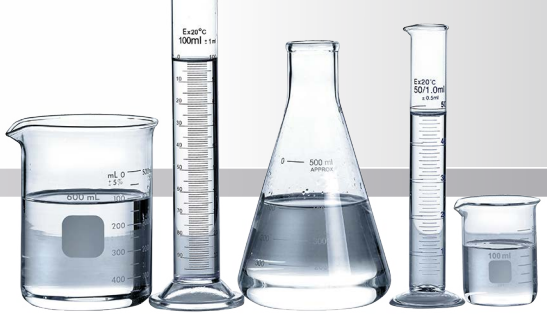
UltiMate 3000 Diode Array and Multiple-Wavelength Detectors

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

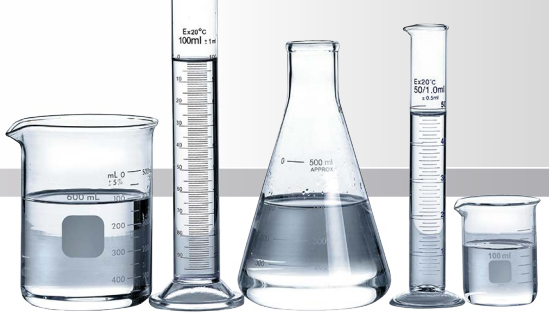
Electrochemical detection delivers high sensitivity for neurotransmitter analysis, simplicity and robustness for pharmaceutical or clinical diagnostics, and the selectivity for the characterization of complex samples such as natural products, biological tissues and fluids. For today's researcher, there 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



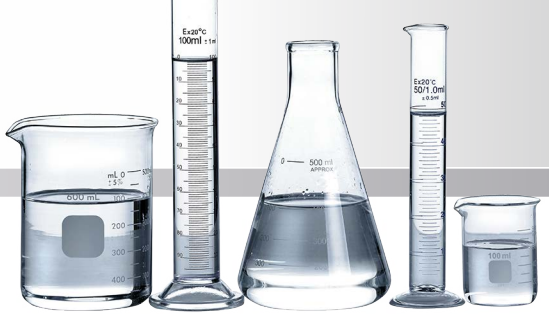
Advanced Detection Capabilities

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.

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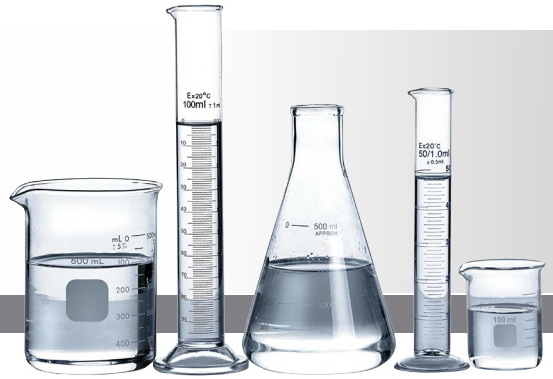
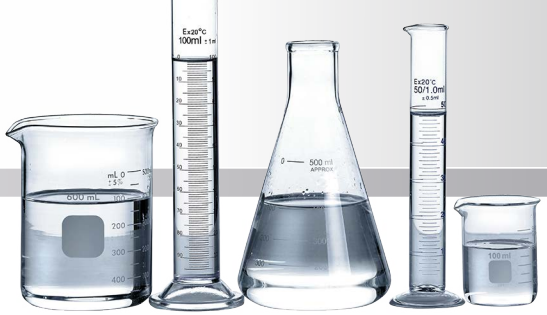


Analytical Technologies

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.



IC and RFIC Systems

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

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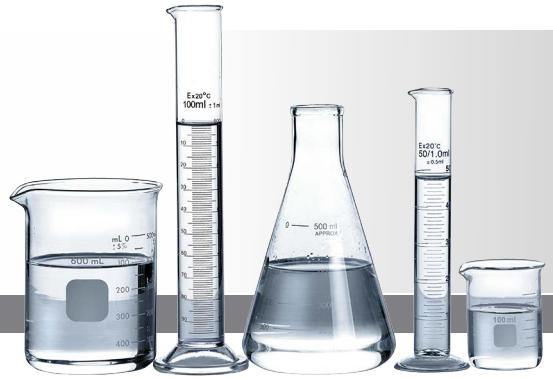
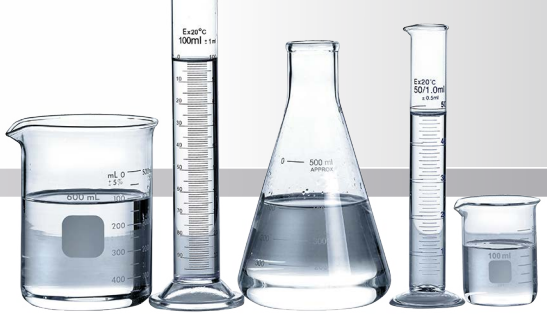


Analytical Technologies

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.



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

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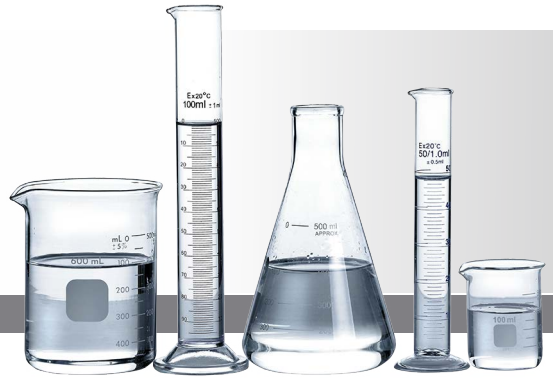

Analytical Technologies

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.

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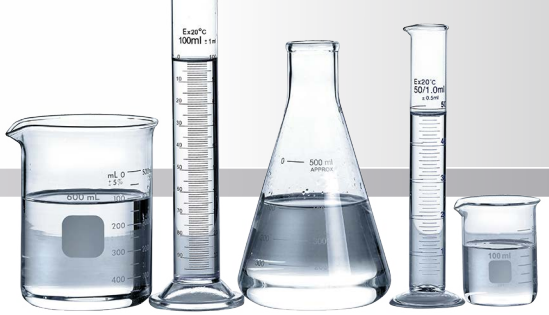

Chromeleon CDS Software

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

Excel is a registered trademark of Microsoft Corporation.

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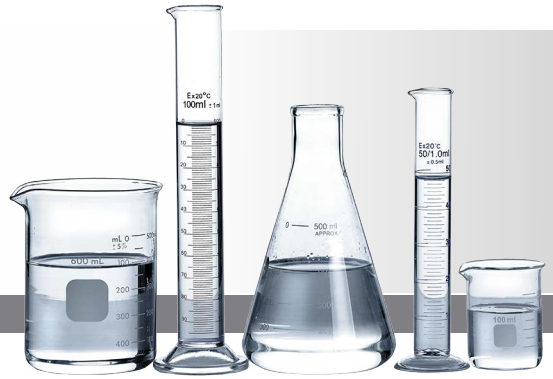

Analytical Technologies

Process Analytical Systems

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

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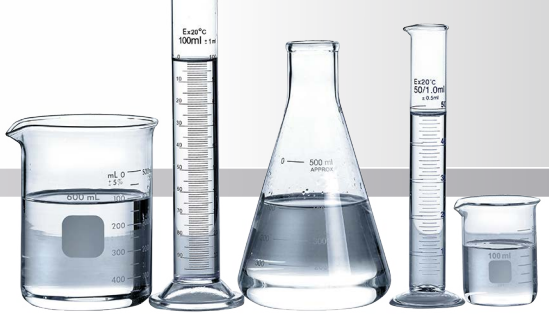

Process Analytical Systems and Software

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

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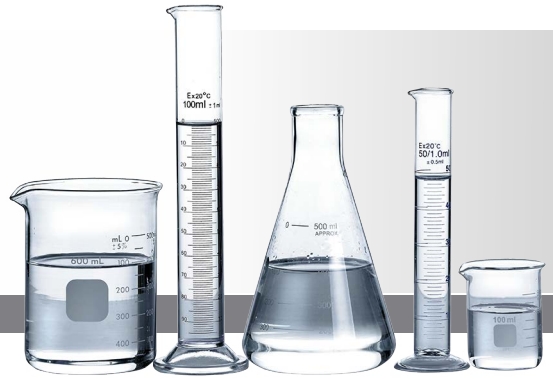

Analytical Technologies

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.

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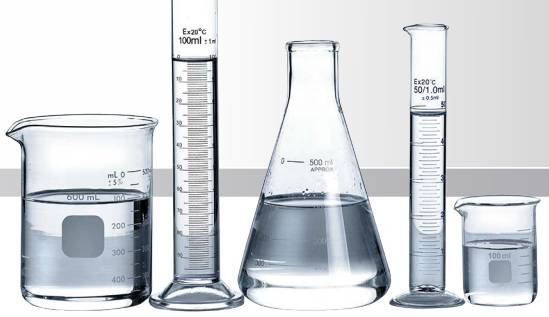


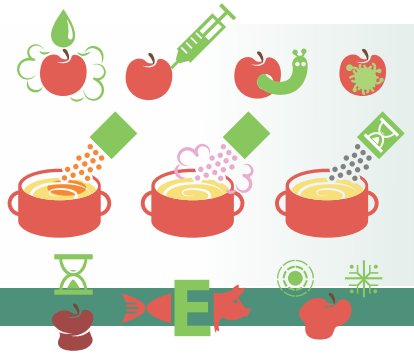
Accelerated Solvent Extractor System

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



Process Contaminants Including Acrolein

Carbonyl compounds are widely found in food products. They can originate from raw materials, alcoholic fermentation, or from a wide range of chemical reactions such as lipid oxidation, Maillard reactions, Strecker degradation, and aldol condensation.

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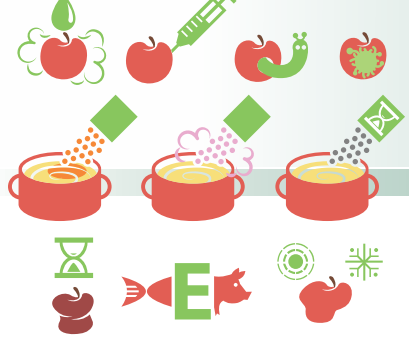

Process Contaminants

Acrolein and Other Carbonyl Compounds

Acrolein is the α,β-unsaturated carbonyl compound also called prop-2-enal or acrylic aldehyde. Acrolein has a high volatility and very high reactivity. The biological effects of acrolein are a consequence of its reactivity towards biological nucleophiles such as guanine in DNA and cysteine, lysine, histidine, and arginine residues in proteins. Acrolein adduction disrupts the function of these biomacromolecules and may result in disease. To evaluate risk assessment, more information on its occurrence needs to be generated. Reported in Method 63558 is an in-house validated method for the determination of a wide range of carbonyl compounds (acrolein [ACR], acetoin [ACET], glyoxal [GLX], methyl-glyocxal [MeGLX], 5-hydroxymethyl-furfural [HMF] and 9-nonenal [NON]) in beer, wine, and potato chips using LC/MS.

Did You Know?

Acrylamide is present in many different foods regularly consumed. For example, it is found in 40 percent of the calories consumed in the average American diet and in foods ranging quite literally from soup to nuts, including baked and fried potatoes, bread, cereals, coffee, crackers, olives, asparagus, prune juice, dried fruit and many others.

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Process Contaminants

LC Conditions

LC Column:	Thermo Scientific™ Accucore™ RP-MS 2.6 µm, 100 × 2.1 mm
Mobile Phase	A: MeOH, B: H2O
Column Oven Temperature:	40 °C
Total Measurement Time:	7 min

MS Conditions

Ionization Method:	APCI
Polarity:	Negative
Scan Type:	Full scan 150–350 *m/z*
Scan Time:	0.2 s
Probe temperature:	350 °C
Needle Voltage:	3.2 kV
Time Range:	1–7 min
Cone Voltage:	15 V

Table 8-1. Gradient program for Figure 8-1.

Time [min]	A%	B%	Flow Rate [µL/min]
0.0	45	55	400
1.0	45	55	400
3.6	86	14	400
4.0	100	0	400
5.9	100	0	400
6.0	45	55	400
7.0	45	55	400

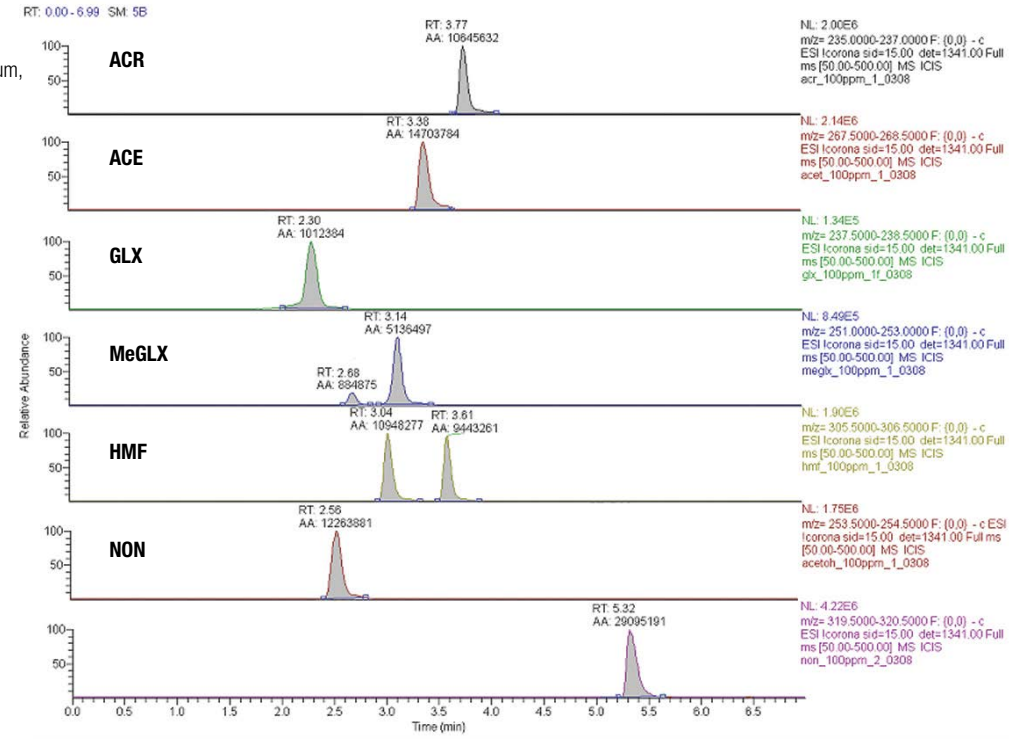
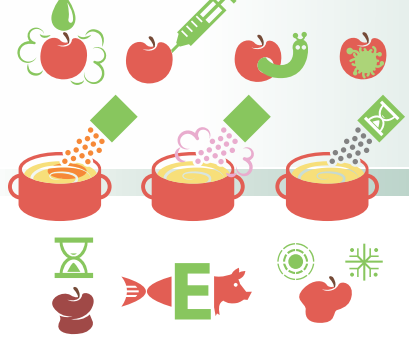


Figure 8-1. Chromatogram of a beer sample spiked at 50 ppm with carbon compounds and after the derivatization reaction. Mass spectrometric detection was carried out by the MSQ single quadrupole mass spectrometer in selected ion monitoring (SIM) mode with atmospheric pressure chemical ionization (APCI). All compounds were individually tuned for optimal cone voltage.



Process Contaminants

Acrolein and Other Carbonyl Compounds

Table 8-2. Method 63558 LOD and LOQ values.

Analyte	Beer		Wine		Chips	
	LOD (mg/kg)	LOQ (mg/kg)	LOD (mg/kg)	LOQ (mg/kg)	LOD (mg/kg)	LOQ (mg/kg)
ACR	0.25	0.8	0.25	0.8	0.25	0.8
ACET	0.6	2	0.6	2	0.6	2
ACETOH (IS)	7.5	25	7.5	25	7.5	25
GLX	6	20	4.5	15	4.5	15
MeGLX	5	17	4.5	15	7.5	25
HMF	0.36	1.2	0.3	1	0.3	1
NON	0.18	0.6	0.18	0.6	0.18	0.6

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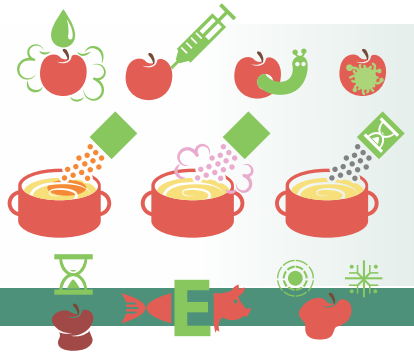
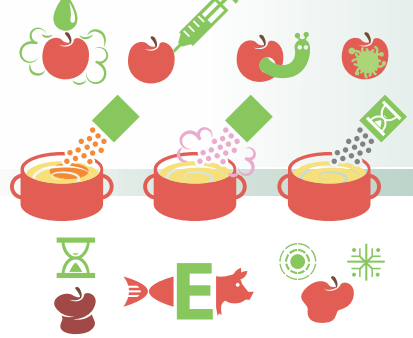


Acrylamide

Acrylamide is a genotoxic compound found in fried or baked goods. It is produced when asparagine reacts with reducing sugars such as fructose or glucose, or carbonyl compounds. Browning the ingredients while cooking produces acylamide, as does overcooking. The acrylamide content in some samples, such as hash browns or french fries, can be particularly high, as much as several mg/kg.



Acrylamide

Methods for acrylamide determination have been published by the U.S. EPA (Method 8032A) using liquid extraction, and by the German Health Agency (BGVV), using HPLC with UV detection. The method presented here demonstrates fast, automated extraction procedure using an Accelerated Solvent Extraction system. The extracts are analyzed by ICE-MS.

The benefits of this method are simplicity and a high degree of automation, which allows analysis of large numbers of samples with minimal labor.

Column:	Dionex IonPac ICE-AS1, 4 × 250 mm,7.5 µm, SP6003
Flow:	0.15 mL/min
Injection Volume:	25 µL
Eluent:	3.0 mM formic acid in acetonitrile/water 30/70 (v/v)
UV Detection:	202 nm
MS Detection:	ESI+: 3.0 kV, cone 50 V, probe temp. 300 °C, scan 50–250 m/z, SIM 72 m/z

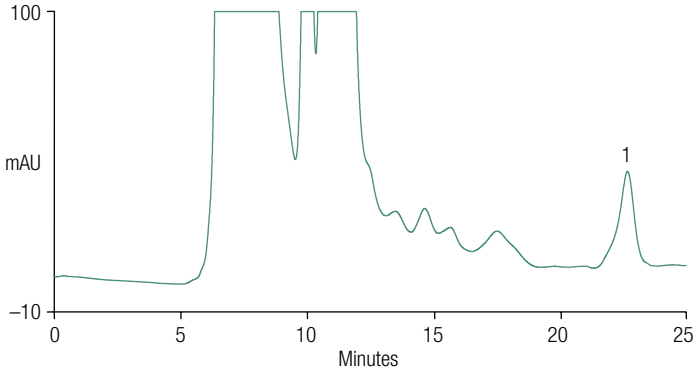


Figure 8-2. Potato chips sample with high acrylamide content.

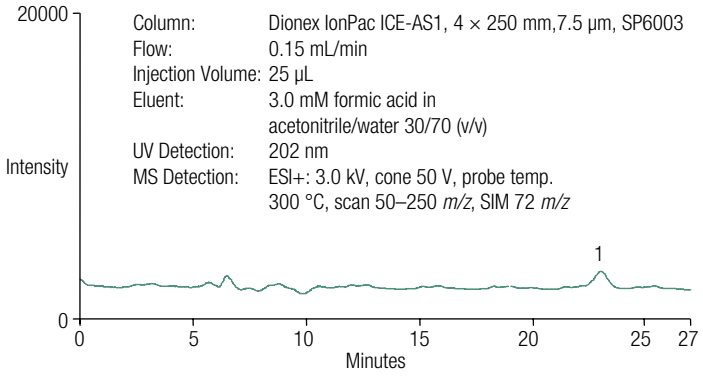
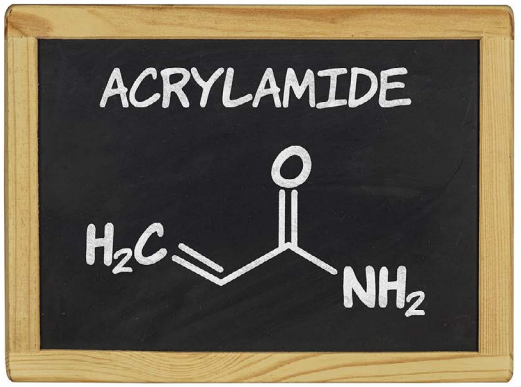


Figure 8-3. SIM chromatogram of crisp bread sample with low acrylamide content.



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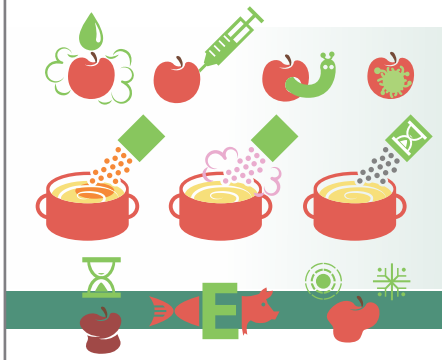
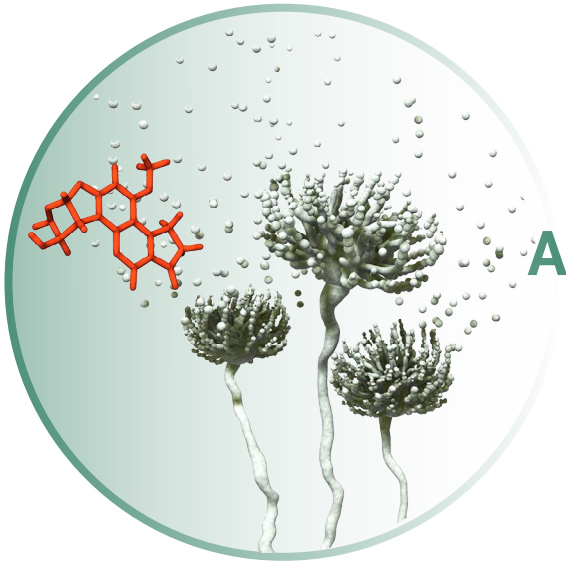
Download Application Note 409: Fast Determination of Acrylamide in Food Samples Using Accelerated Solvent Extraction Followed by Ion Chromatography with UV or MS Detection





Aflatoxins

The fungus *Aspergillus* grows in soil and decaying vegetation, and can colonize and contaminate crops with aflatoxins before harvest or during storage. Aflatoxins are toxic and highly carcinogenic substances, and the presence of aflatoxins B1, B2, G1, and G2 in a variety of processed and unprocessed foods is regulated in countries around the world.

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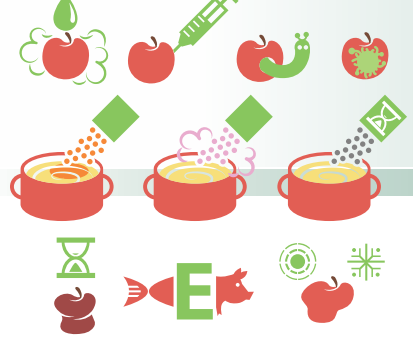


Aflatoxins

The European Commission has set maximum levels for aflatoxin B1 between 2.0 and 8.0 µg/kg and for the sum total of all four of these toxins between 4.0 and 15.0 µg/kg in crops such as nuts, groundnuts, grains, and dried fruits. The U.S. Food and Drug Administration has set action levels (levels where the FDA will take legal action to remove products from the market) of 20 ppb (µg/kg) for the sum total of the four aflotoxins in foods such as corn, peanuts, brazil nuts, and pistachios as well as other foods.

The traditional method for aflatoxins analysis in grains includes soxhlet extraction, sample clean-up using SPE, and separation, identification, and quantification by HPLC. Because of the time-consuming extraction and clean-up steps, sample throughput is limited using this technique. This can be improved by using an accelerated solvent extraction system followed by on-line SPE-LC.

The extract was analyzed by on-line solid-phase extraction coupled to a high-performance liquid chromatographic system (online SPE-LC). The UltiMate ×2 Dual-Gradient HPLC system was used, comprising a six channel on-line degasser; two integrated gradient pumps used for sample loading, sample cleanup, and separation on the analytical column; a cooled well-plate autosampler with split loop injection; a thermostatted column compartment equipped with a 6-port switching valve; a photochemical derivatizer; and a fluorescence detector.

The stationary phase of the Venture™ AF SPE immunoaffinity 15–20 µm 50 × 2.1 mm column selectively retained the target analytes (aflatoxins) from the sample matrix. The enriched analytes were transferred in a back-flush mode to an Acclaim 120 C18 3 µm, 4.6 × 150 mm column for the reversed-phase separation of the B1, B2, G1, and G2 aflatoxins.

After separation, the aflatoxins B1 and G1 were photochemically derivatized by irradiation with UV light at 254 nm, allowing detection of these aflatoxins with a fluorescence detector. The photochemical derivatization has no influence on the chemical or measurement related properties of aflatoxins B2 and G2.

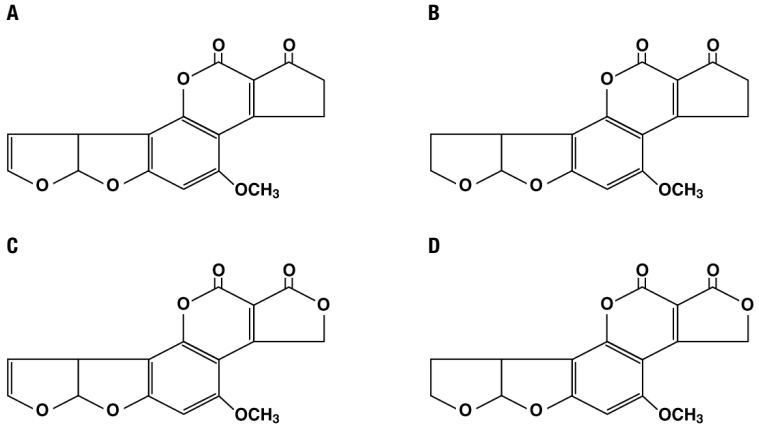
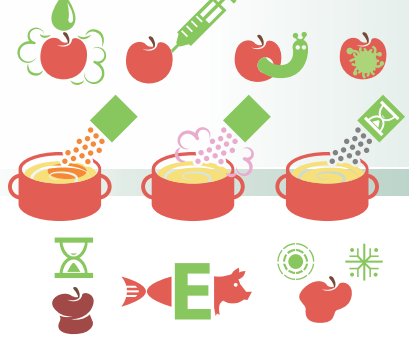


Figure 8-4. Molecular structures of aflatoxins: (A) Aflatoxin B1, (B) Aflatoxin B2, C) Aflatoxin G1, and (D) Aflatoxin G2.

Download Poster Note: Fast and Effective Determination of Aflatoxins in Grains or Food Using Accelerated Solvent Extraction followed by HPLC



Aflatoxins

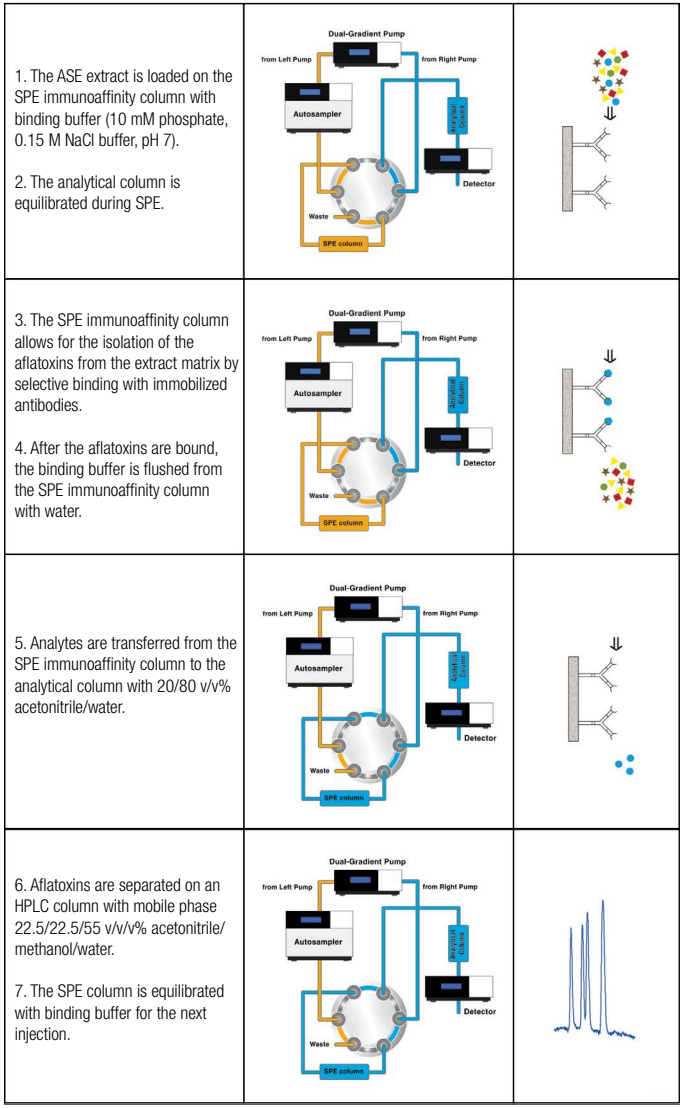


Figure 8-5. This figure shows the various steps in the on-line sample preparation and detection of aflatoxins B and G.

Table 8-3. Program events during on-line SPE-LC analysis.

Time (min)	Valve Position	Loading Solvent for SPE Column, 250 µL/min A) Binding buffer B) Water	Transfer/Elution for Analytical Column, 1.00 mL/min A) 20/80 CH_3CN/H_2O B) 22.5/22.5/55 $CH_3OH/ CH_3CN/H_2O$
0.0	1_2	100% A	100% A
5.0		100% A	100% A
5.1		100% B	100% A
10.0	6_1	100% B	100% A
10.1		100%A	100% A
14.5		100%A	100% A
14.6	1_2	100%A	100% B
27.6		100%A	100% B
27.7		100%A	100% A
40.0		100%A	100% A

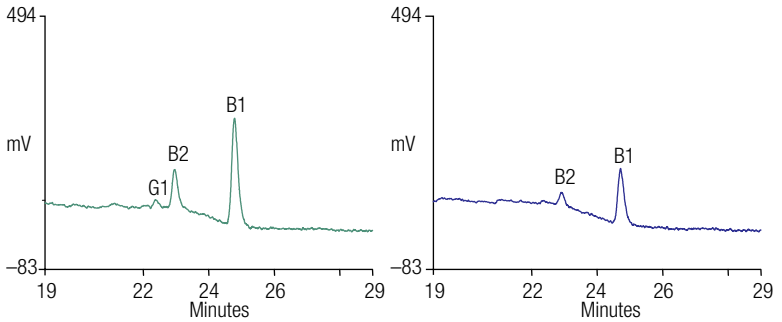


Figure 8-6. Chromatogram of aflatoxin determination by SPE-LC in almond (left) and corn (right).

Table 8-4. Amount of aflatoxins found in almond and corn samples.

Compound	Almond Amount (µg/kg)	Corn Amount (µg/kg)
G2	<LOD	<LOD
G1	3	<LOD
B2	6	1
B1	53	27

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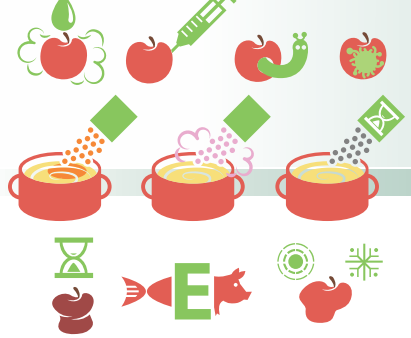


Aflatoxins and Ochratoxin A

The production of herbal supplements and spices is a fast growing industry. Unfortunately, the raw materials are often imported from countries that lack adequate quality control and whose weather conditions during the growing season, along with improper harvesting and storage practices, can cause toxic mold contamination. There are numerous reports on the presence of Mycotoxins in commercially available herbs and spices such as chamomile, black and white tea leaves, ginkgo leaves, paprika, and cumin.

A simple, sensitive, and robust HPLC method for determining Aflatoxins B1, B2, G1, G2, and Ochratoxin A in herbs and spices was developed. Afla-OtaCLEAN™ (LCTech, Germany) Immunoaffinity columns containing antibodies specific for both classes of Mycotoxins allowed for fast and efficient sample clean-up. Post-column photochemical derivatization was used to increase the sensitivity of detection of Aflatoxins B1 and G1. The UVE™ (LCTech, Germany) photochemical reactor requires no additional reagents and was installed between the HPLC column and fluorescence detector. Ochratoxin A is a naturally fluorescent compound that does not require derivatization and can be determined together with all four Aflatoxins.

Column:	C18, 4.6 × 250 mm		
Flow:	1 mL/min		
Injection Volume:	30 µL		
HPLC Eluent:	Sodium Phosphate buffer (Pickering Laboratories Inc. Cat #1700-1108), Methanol, Acetonitrile		
HPLC Gradient:			
Time (min)	Sodium Phosphate (%)	Methanol (%)	Acetonitrile (%)
0	57	28	15
13	57	28	15
13.1	40	60	0
23	40	60	0
23.1	0	100	0
28	0	100	0
Equilibration:	12 min		
FLD:	Excitation 365 nm, Emission 430 nm for Aflatoxins (0–16 min) Excitation 335 nm, Emission 455 nm for Ochratoxin A (16–28 min)		

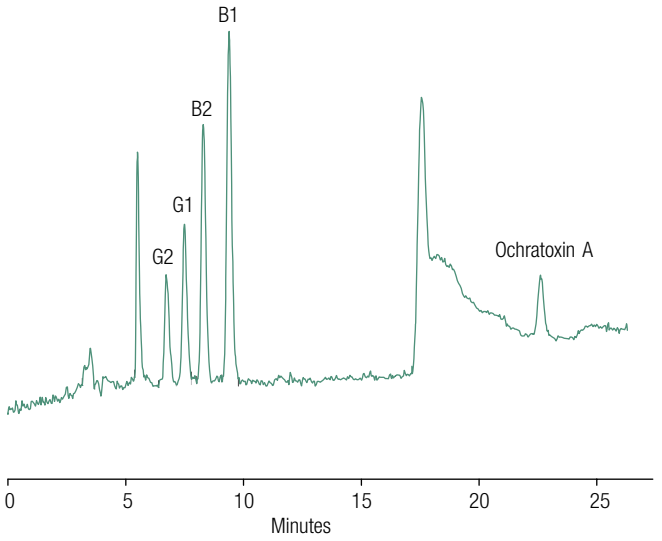
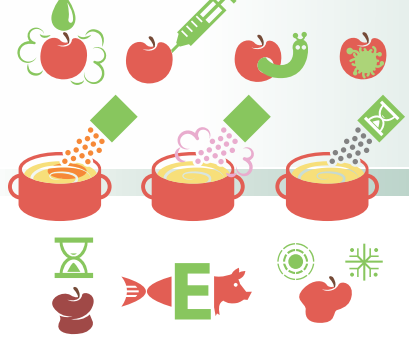


Figure 8-7. Ginger sample spiked with mycotoxins: Aflatoxin B1 ,5.06 ng/g; Aflatoxin B2, 1.45 ng/g; Aflatoxin G1, 4.33 ng/g; Aflatoxin G2, 1.45 ng/g; Ochratoxin A, 10.1 ng/g.



Aflatoxins and Ochratoxin A

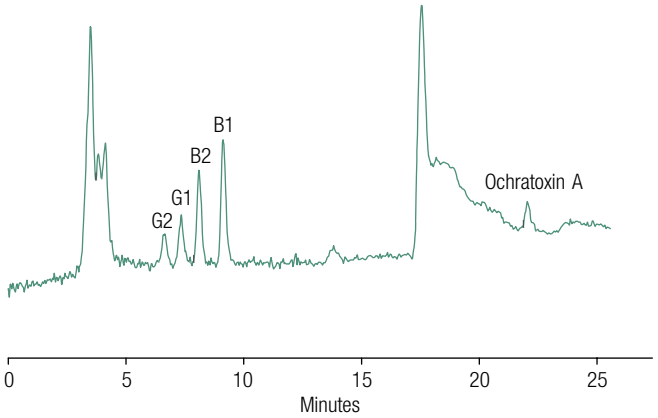


Figure 8-8. Ginseng sample spiked with mycotoxins: Aflatoxin B1, 2.53 ng/g; Aflatoxin B2, 0.72 ng/g; Aflatoxin G1, 2.16 ng/g; Aflatoxin G2, 0.72 ng/g; Ochratoxin A, 5.05 ng/g. For conditions see Figure 8-7.

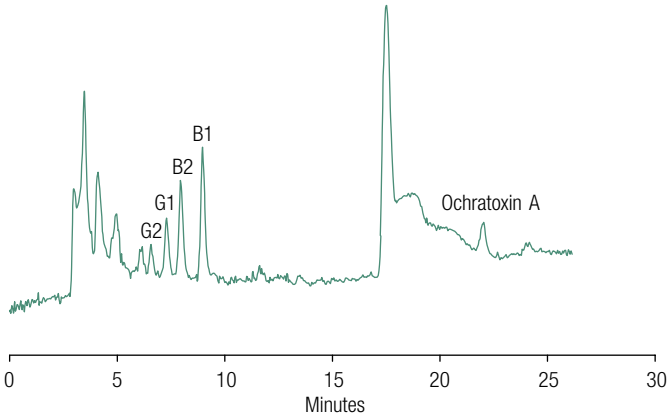


Figure 8-9. Echinacea sample spiked with mycotoxins: Aflatoxin B1, 2.53 ng/g; Aflatoxin B2, 0.72 ng/g; Aflatoxin G1, 2.16 ng/g; Aflatoxin G2, 0.72 ng/g; Ochratoxin A, 5.05 ng/g. For conditions see Figure 8-7.

Triva Question

Q: Do you know how many types of aflatoxin are produced in nature?

A: 14 different types of aflatoxin are produced in nature, with Aflatoxin B1 being the most toxic.

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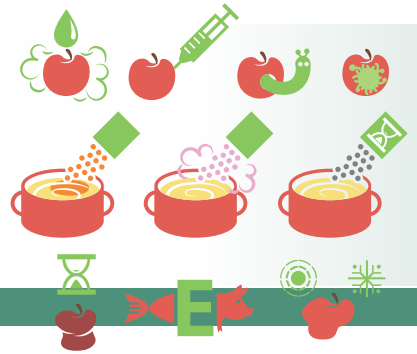

Aniline and Nitroanilines

Aniline is an organic compound widely used in the polymer, rubber, pharmaceutical, and dye industries. Aniline and its derivatives (e.g., nitroanilines) are suspected carcinogens and are highly toxic to aquatic life. Therefore, it is necessary to establish sensitive, efficient, and simple methods for the determination of aniline and its derivatives in drinking and environmental waters.

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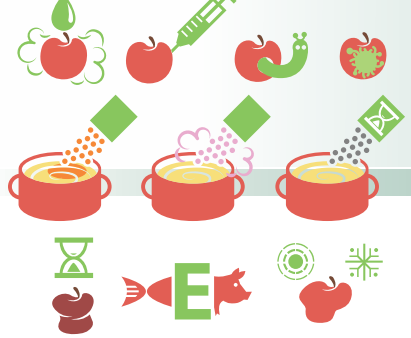


Aniline and Nitroanilines

Aniline and Nitroanilines in Drinking Water

Normally, extraction processes for aniline and its derivatives from environmental and drinking water samples prior to HPLC analysis are required due to the limited sensitivity of direct injection for these samples, which have low concentrations of anilines. The typical extraction techniques are liquid-liquid extraction and solid-phase extraction (SPE), with SPE gaining favor either in the on-line or off-line mode. Compared to off-line SPE, on-line SPE offers the advantages of full automation, absence of operator influence, time savings, and strict process control.

Application Note 292 describes an on-line SPE HPLC system for the simple and sensitive determination of aniline and four nitroanilines—*o*-nitroaniline, *m*-nitroaniline, *p*-nitroaniline, and *o,p*-dinitroaniline—in tap and pond water.

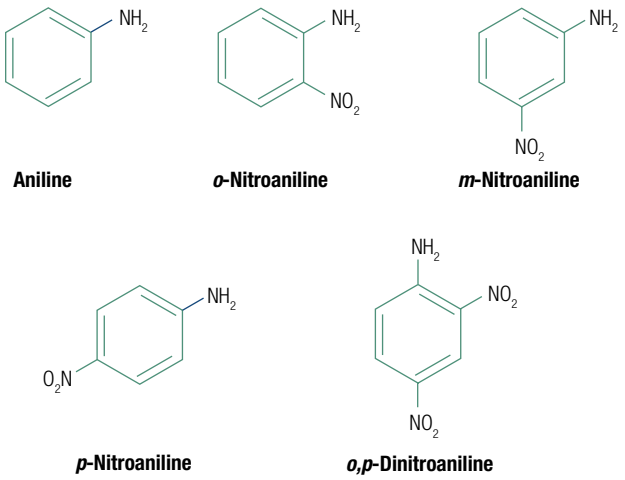


Figure 8-10. Structures of aniline and nitroanilines.

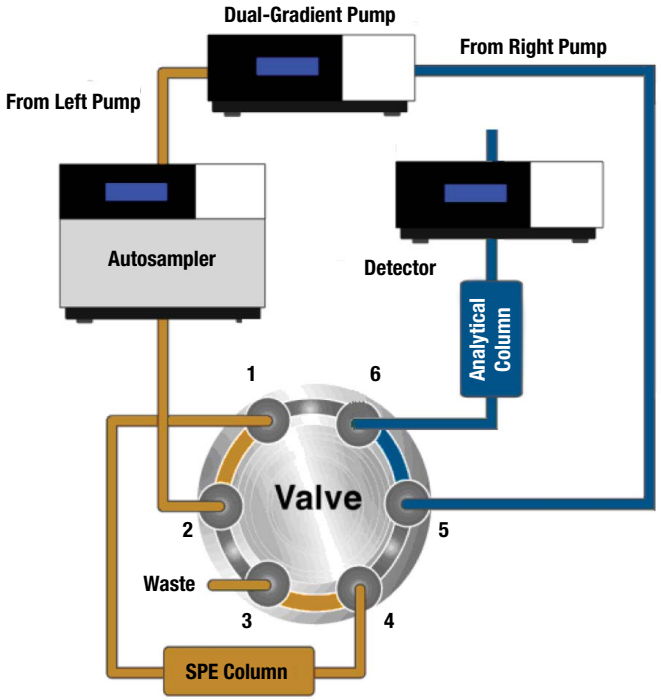
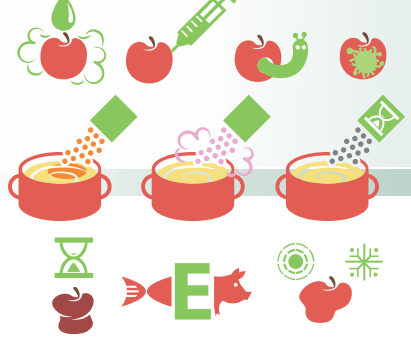


Figure 8-11. Flow schematic of on-line SPE.



Aniline and Nitroanilines

Analytical Column:	Thermo Scientific™ Acclaim™ 120 C18 (3 µm, 4.6 × 150 mm)
SPE Cartridge:	Thermo Scientific™ Dionex™ SolEx™ SPE Cartridges HRP (12–14 µm, 2.1 × 20 mm)
Flow:	For on-line SPE: 0~2 min, 2.0 mL/min; 3~10 min, 0.5 mL/min; 11~15 min, 2 mL/min For separation: 1.0 mL/min
Column Temp.:	30 °C
Injection Volume:	5000 µL on the on-line SPE cartridge (two consecutive injections of 2500 µL using UDP injection mode)
Mobile Phase:	For on-line SPE: 10 mM phosphate buffer (pH 6.5)/CH_3OH, In gradient: CH_3OH, 0~2 min, 10%; 3~10 min, 70%; 11~15 min, 10% For separation: H_2O/CH_3CN In gradient: CH_3CN, 0~2 min, 30%; 10 min, 55%; 11~13 min, 70%; 15 min, 30%
UV Detection:	Absorbance at 230 nm

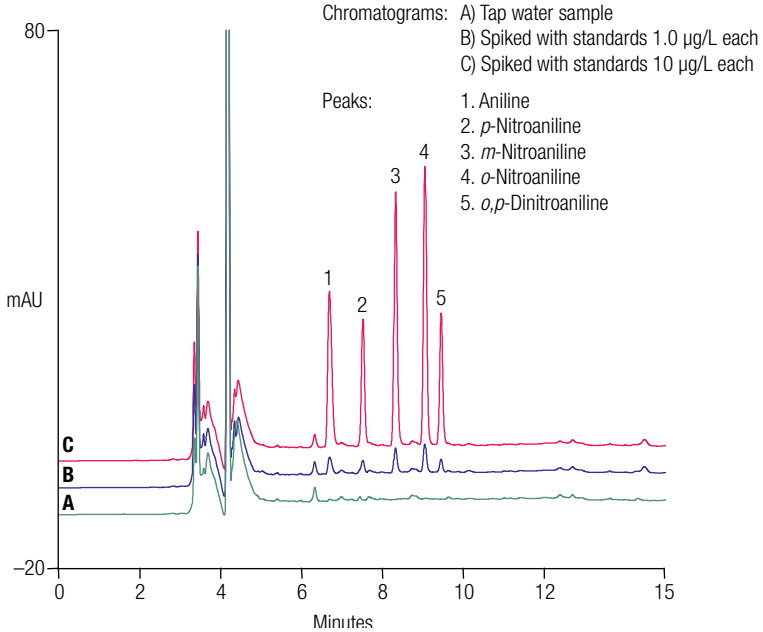


Figure 8-12. Chromatograms of (A) tap water sample, (B) the same sample spiked with 1.0 µg/L aniline and nitroanilines standard, and (C) spiked with 10 µg/L.

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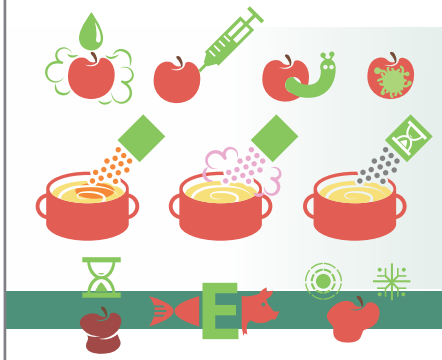
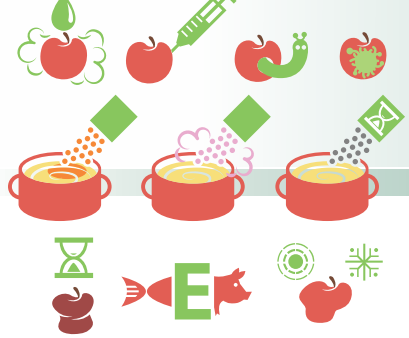


Antibtiotics

The use of antibiotics on livestock, aquaculture, and bee husbandry helps maintain health and provides other benefits such as improved disease resistance, increased production, and in some cases, reduction in foodborne pathogens. However, antibiotic residues in foods can cause undesirable side effects such as idiosyncratic aplastic anemia, production of antibiotic-resistant bacteria, and the reduction of indigenous microbiota found in the human digestive tract. In addition, the wastes of these animals can lead to antibiotics being present in our water.



Antibtiotics in Feed

Organizations responsible for food safety perform assays for the presence of allowed and banned antibiotics as part of their surveillance activities. This application demonstrates a reproducible RSLC method for the separation of polyketide (tetracycline and oxytetracycline), macrolide (tylosin), phenicol (chloramphenicol), nitrofuran (nitrofurantoin), and sulfonamide (sulfathiazole) classes of antibiotics with an MS-compatible mobile phase.

Column:	Acclaim RSLC Polar Advantage II, 2.2 µm, Analytical (2.1 × 150 mm)					
Flow:	0.8 mL/min					
Temperature:	30 °C (Autosampler: 5 °C)					
Injection Volume:	10 µL					
Mobile Phases:	A) 0.5% Formic acid in water					
	B) 0.5% Formic acid in acetonitrile					
Gradient Time (min):	0	2	4	4.1	5.9	6
%A	90	74	48	10	10	90
%B	10	26	52	90	90	10
Detection:	Absorbance, UV at 267 nm					

Peaks:	1. Sulfathiazole	10 µg/mL
	2. Oxytetracycline	10
	3. Tetracycline	10
	4. Nitrofurantoin	10
5 (a,b,c).	Tylosin and related products	10
	6. Chloramphenicol	10

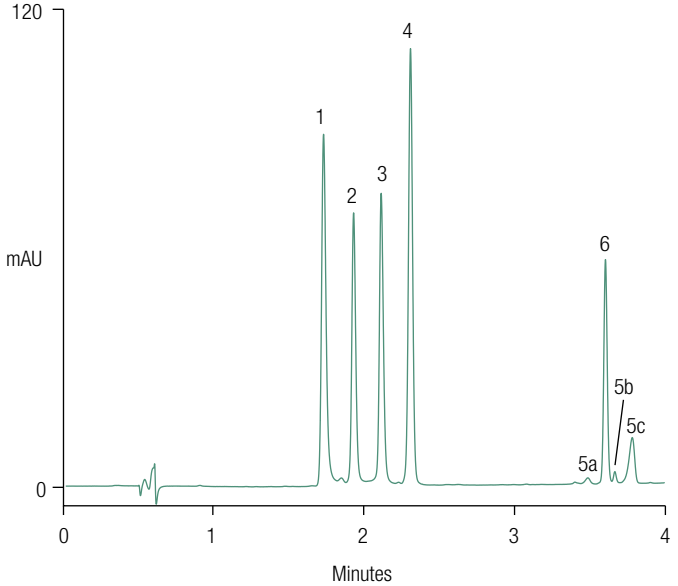
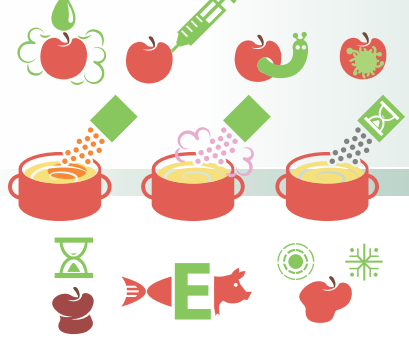


Figure 8-13. Separation of multiple classes of antibiotics using the UltiMate RSLC system and UV-diode array detection at 267 nm.



Antibtiotics in Feed

Antibiotics in Distiller's Grain

Distiller's grain (DG), a major coproduct of dry-grind ethanol processing, quadrupled in production during 2004–2005. DG is a valuable product to the livestock industry because it is a rich source of protein, fat, minerals, and vitamins, thus making it an excellent feed supplement for livestock and poultry. However, bacterial contamination from lactic acid-producing bacteria—such as *Lactibacillus, Lueconostoc,* and *Weissella*—is a concern for ethanol production facilities because bacteria compete with yeast for sugar and micronutrients. Antibiotics such as virginiamycin, penicillin, and erythromycin are commonly used during fermentation to inhibit bacterial growth. The FDA has raised concern over food producing animals consuming DGs with antibiotic residues, and how this may lead to increased antibiotic resistance in humans and animals. Therefore, to assess the amount of antibiotics in DGs and to meet possible future regulatory requirements, analytical methods are needed to determine residual antibiotics in DGs. This method allows the determination of penicillin G, erythromycin, and virginiamycin S1 and M1 in dried distillers grains with solubles (DDGS).

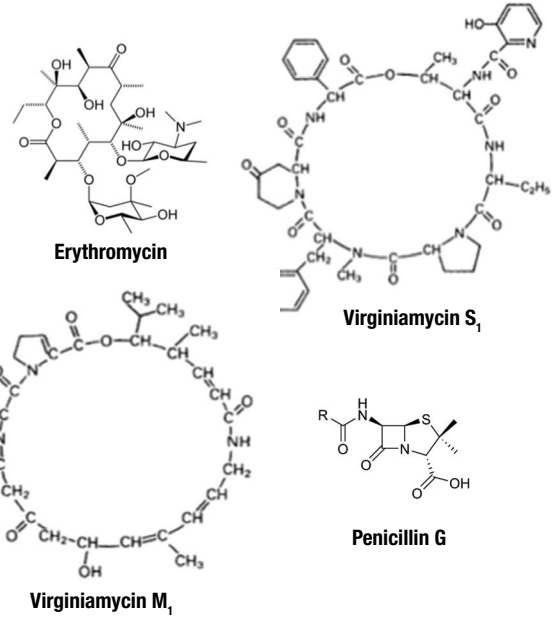
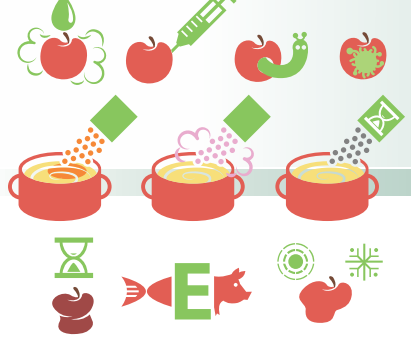


Figure 8-14. Structures of antibiotics used in the ethanol production process.

Did You Know?

Antibiotics are given to livestock for two reasons: to promote animal health, and to make animals grow faster. Food animals get 80% of the antibiotics used in the U.S. 15,000 tons of antibiotics are used in U.S. to treat food animals each year.

Download Application Note 1055: Determination of Virginiamycin, Erythromycin, and Penicillin in Dried Distillers Grains with Solubles



Antibtiotics in Feed

Column:	Acclaim 300 C18, 3 µm, Analytical (2.1 × 150 mm)
Flow:	0.75 mL/min
Temperature:	25 °C
Injection Volume:	10.0 µL
Eluent:	A: 0.025% HFBA in 25% CH_3CN B: Ethyl Acetate C: 0.025% HFBA in CH_3CN
Gradient:	0.0–3.0 min 100% A, 3.0–19.0 min 1.0% B/75% C, hold at 1.0% B/75% C for 1 min, step change at 20.0 min 100% A, hold at 100% A for 5 min
Detection:	Charged Aerosol, low filter, 60 Hz data collection rate, nebulizer temperature 15 °C
Sample:	Mixed Antibiotic Standard

Peaks:

1. Penicillin	50.0 µg/mL
2. Erythromycin	50.0
3. Virginiamycin M_1	50.0
4. Virginiamycin S_1	50.0

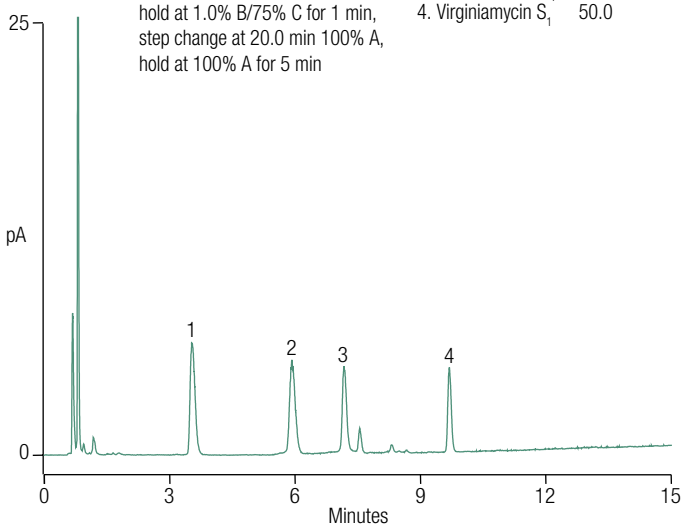


Figure 8-15. Chromatogram showing the separation of a mix of four antibiotics on the Acclaim 300 C18 column using charged aerosol detection.

Column:	Acclaim 300 C18, 3 µm, Analytical (2.1 × 150 mm)
Eluent:	A: 0.025% HFBA in 25% CH_3CN B: Ethyl Acetate C: 0.025% HFBA in CH_3CN
Gradient:	0.0–3.0 min 100% A, 3.0–19.0 min 1.0% B/75% C, hold at 1.0% B/75% C for 1 min, step change at 20.0 min 100% A, hold at 100% A for 5 min
Flow Rate:	0.75 mL/min
Inj. Volume:	10.0 µL
Temperature:	25 °C
Detection:	Charged Aerosol, low filter, 60 Hz data collection rate, nebulizer temperature 15 °C
Samples:	(A) Unspiked DDGS (B) Spiked DDGS

Peaks:

1. Penicillin	12.5 µg/mL
2. Erythromycin	12.5
3. Virginiamycin M_1	12.5
4. Virginiamycin S_1	12.5

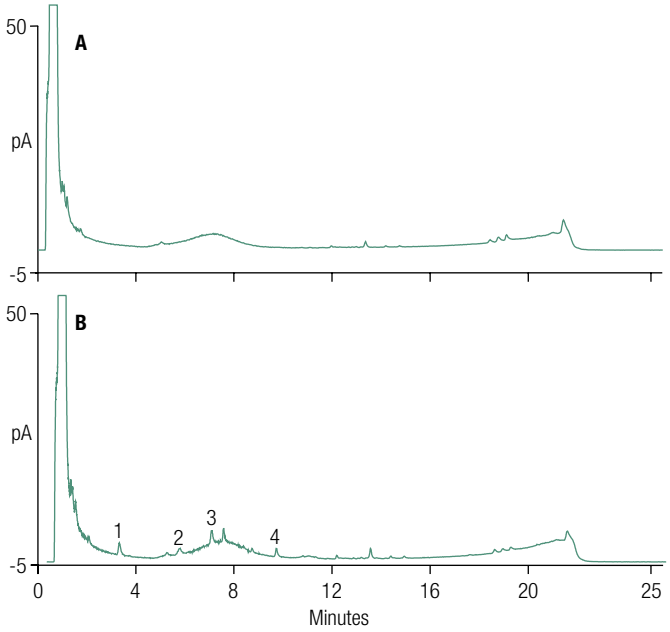
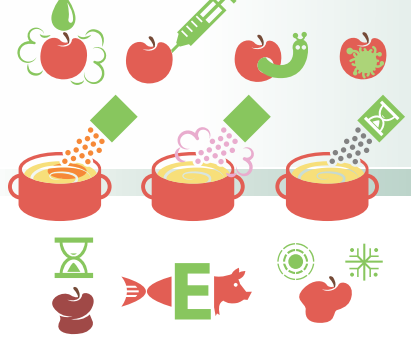


Figure 8-16. Chromatograms showing the separation of (A) an unspiked DDGS sample and (B) a DDGS sample spiked with a mix of the four antibiotics using the Acclaim 300 C18 column with charged aerosol detection.



Antibtiotics in Feed

Nitrofuran Antibiotics in Animal Feed

Column:	Acclaim 120 C18, 5 µm, 4.6 × 150 mm
Flow:	1.0 mL/min
Temperature:	30 °C
Injection Volume:	20 µL
Mobile Phase:	Acetonitrile:10 mM ammonium acetate pH 5.0, 20:80 v/v; isocratic
Detector:	Summit UVD340U diode array, 365 nm, and spectra 200–500 nm
Sample Prep.:	1. 3.0 g guinea pig feed in a 50 mL centrifuge tube 2. Add 9 mL water and let stand 5 min. 3. Add 21 mL methanol:acetonitrile 1:1 and extract for 30 min. 4. Pass through cleanup cartridge containing 1.7g of neutral alumina; discard first 1.7 mL, retain next 3.5 mL
Peaks:	1. Nitrofurazone 2. Nitrofurantoin 3. Furazolidone 4. Furaltadone

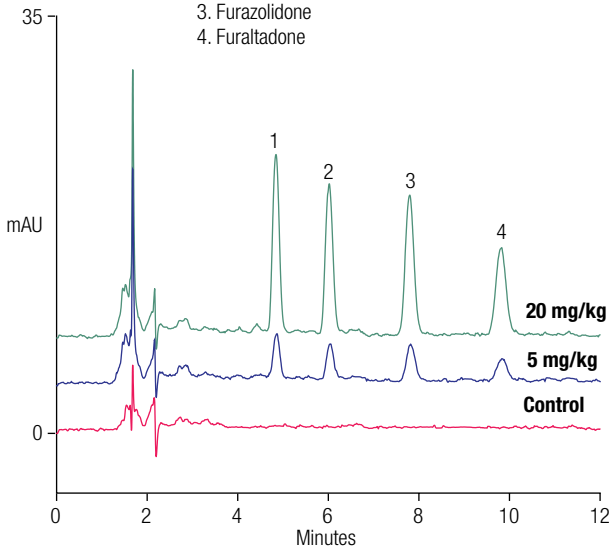


Figure 8-17. Nitrofuran antibiotic residues in animal feed on the Acclaim 120 C18 column.

Ionophore Antibiotics in Animal Feed

Antibiotics can be categorized based on their chemical structure, including: beta-lactams, aminoglycosides, tetracyclines, fluoroquinolines, macrolides, and polyether ionophores. The use of polyether ionophorous antibiotics (monensin, salinomycin, lasolacid A, and narasin) in industrial agriculture is significant, with over 3,700,000 kg approved for use in 2009 by the Food and Drug Administration. Ionophores are approved feed additives, and are used to a large extent in the poultry and beef production industry to control and prevent coccidiosis disease. Adding these ionophores to animal feeds can improve growth rates, but there is concern that antibiotic residues may remain in tissues, food products, and the environment.

Some animals such as horses, certain avian species, dogs, and cats are especially sensitive to ionophore toxicity. Thus, there is a need for sensitive methods for their analysis. Presented here is a gradient HPLC-charged aerosol detector method capable of measuring a number of ionophore antibiotics.

HPLC System:	UltiMate 3000 RSLC DGP
HPLC Column:	Acclaim RSLC 120 C18, 2.2 µm, 2.1 × 250 mm
Flow:	0.50–0.85 mL/min
Column Temp.:	50 °C
Injection Volume:	10 µL
Mobile Phase:	A: Water/methanol (350:650), 0.1% acetic acid B: Methanol, 0.1% acetic acid
Sample Solvent:	Water/methanol (9:91)
Sample Temp.:	15 °C

Gradient:

Time (min)	Flow Rate (mL/min)	%A	%B
-3.0	0.55	100.0	0.0
0.0	0.50	100.0	0.0
0.5	0.50	100.0	0.0
1.0	0.50	58.0	42.0
2.0	0.51	56.5	43.5
4.0	0.56	50.0	50.0
10.0	0.56	45.0	55.0
23.0	0.65	45.0	55.0
26.0	0.65	37.0	63.0
28.0	0.65	0.0	100.0
33.0	0.85	0.0	100.0
33.0	0.85	100.0	0.0
35.0	0.55	100.0	0.0

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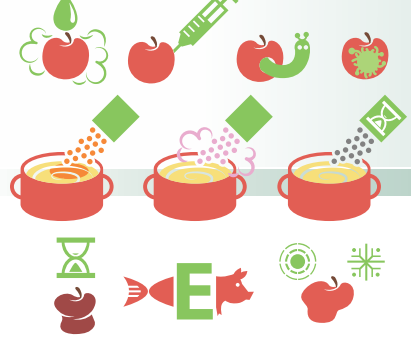

Antibiotics in Meat

Chicken

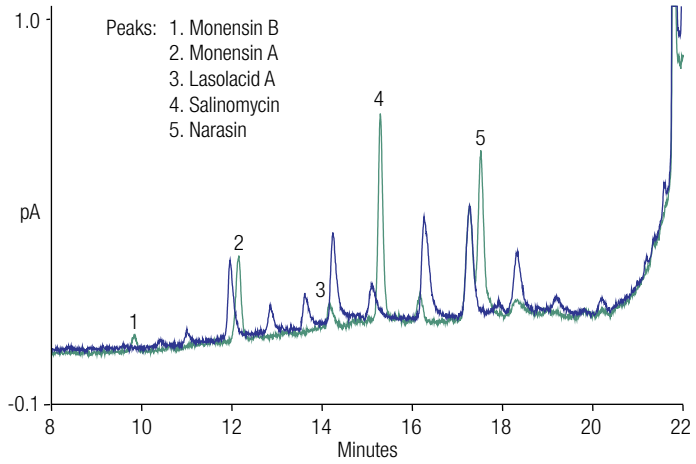

Figure 8-18. Chicken meat extract blank chromatogrm (purple), overlaid with ionophore standard chromatogram (19 ng o.c.) (green).

Pork

Column:	Acclaim PA C18 5 µm, 4.6 × 150 mm			
Flow:	1.5 mL/min			
Temperature:	30 °C			
Injection Volume:	60 µL			
Mobile Phase:	(A) 22 mM H_3PO_4, 0.5 mM $Na_4P_2O_7$			
	(B) Acetonitrile			
Gradient:	Time	0.0	0.5	7.0
	%A	82	82	45
	%B	18	18	55
Detector:	UVD 340U, UV at 360 nm			
Samples:	(A) Spiked pork muscle,1.0 µg/g each			
	(B) Control pork			
	(C) Tetracycline standards, 0.33 µg/mL in water			

Sample Prep.:
- 2.0 g pork muscle tissue
- Grind with mortar and pestle in sequence with 0.1 g of citric acid
  1.0 mL of 3.6 M HNO_3
  4.0 mL of methanol
  1.0 mL of water
- Centrifuge

Peaks:
1. Oxytetracycline
2. Tetracycline
3. Chlortetracycline
4. Doxycycline

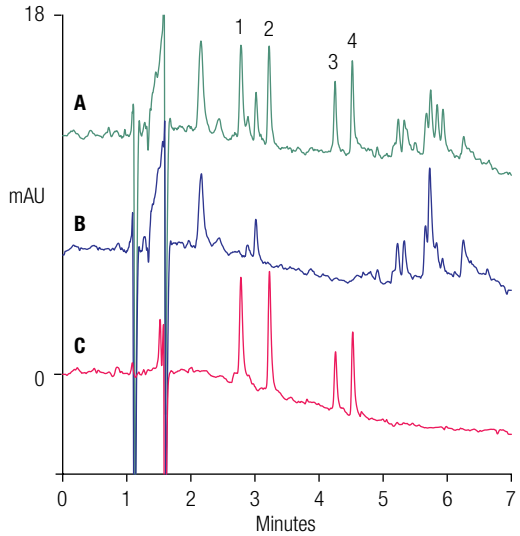

Figure 8-19. Tetracyclines in pork using the Acclaim PA column.

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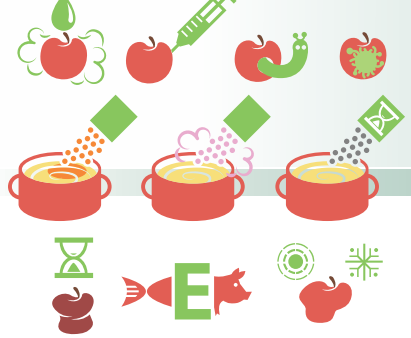
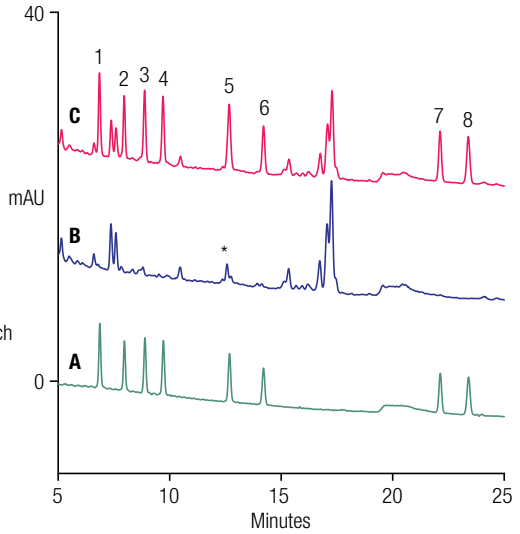


Antibiotics in Milk

Sulfonamide antibiotics, some approved and some banned, are used in veterinary medicine to treat dairy cattle. Maximum contamination levels have been established for milk. The conventional assay requires two injections with different mobile phases to all compounds listed below. This improved method using a high resolution Acclaim 120 C18 column with gradient elution can resolve the entire list.

Column:	Acclaim 120 C18 5 µm, 4.6 × 250 mm
Flow:	1.5 mL/min
Temperature:	35 °C
Injection Volume:	100 µL
Mobile Phase:	(A) 30 mM acetic acid adjusted to pH 4.2 with NaOH (B) Methanol
Gradient:	Time 0.0 20 25 %A 88 60 60 %B 12 40 40
Detector:	UVD 340U, UV at 265nm with spectral confirmation
Sample Prep.:	AOAC 993.32; refer to procedure for important notes
Samples:	(A) Spiked extract of skim milk,1.0 µg/g each (B) Milk extract (C) Sulfonamide standards, 0.20 µg/mL in water
Peaks:	1. Sulfadiazine (SDZ) 2. Sulfathiazole (STZ) 3. Sulfapyridine (SPD) 4. Sulfamerazine (SMR) 5. Sulfamethazine (SMZ) 6. Sulfachloropyridazine (SCP) 7. Sulfadimethoxine (SDM) 8. Sulfaquinoxzline (SQX) *. Theobromine



Note: Most interferences are organic acids that may be moved out of the way by small adjustements to the pH of the mobile phase

Figure 8-20. Sulfonamide antibiotic residues in milk using the Acclaim 120 C18 column.

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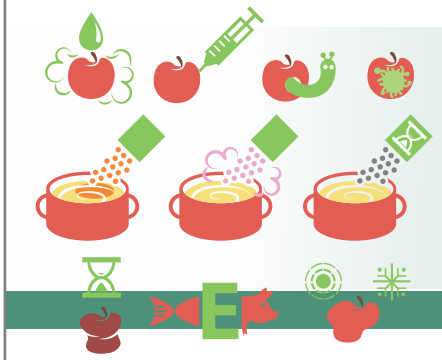

Aristolochia

Aristolochia species (e.g., Virginia snakeroot, guaco) are common ingredients in traditional Chinese herbal remedies and herbal dietary supplements. Unfortunately, over the last ten years consumption of herbals containing *Aristolochia* has resulted in numerous cases of late stage renal failure often associated with urothelial tract carcinoma.

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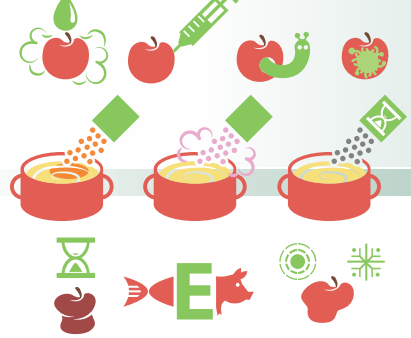


Aristolochia

"Chinese herbs neuropathy", the disease resulting from consumption of *Aristolochia*, has now been renamed "aristolochic acid nephropathy" in recognition of the active toxin(s) present and the fact that *Aristolochia* species are used in many non-Chinese herbal supplements. In 2000, the FDA released a warning to health care professionals warning of the consequences of *Aristolochia* consumption.

The principal nephratoxin present is aristolochic acid (AA). AA is actually composed of a group of several nitrophenanthrene carboxylic acids, aristolochic acid I (AA1) and aristolochic acid II (AA2) being the most abundant. Neither AA1 nor AA2 are toxic *per se*. However, upon metabolic activation they form reactive intermediates that are capable of damaging DNA.

Column:	Acclaim120 C18, 3 µm Analytical, 3 × 150 mm
Flow:	1 mL/min
Temperature:	30° C
Injection Volume:	5 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:	-5 - 0 min, 50% B, 3% C; 10 min, 97% B, 3% C; 20 min, 97% B, 3% C.
UV Detection:	Channel 1, 218 nm; Channel 2, 250 nm; Channel 3, 302 nm; Channel 4, 321 nm
EC Detection:	6 Channel Array from +600 to +900 mV, relative to Pd, in 60 mV increments
Peaks:	1. Aristolochic Acid II 2. Aristolochic Acid I

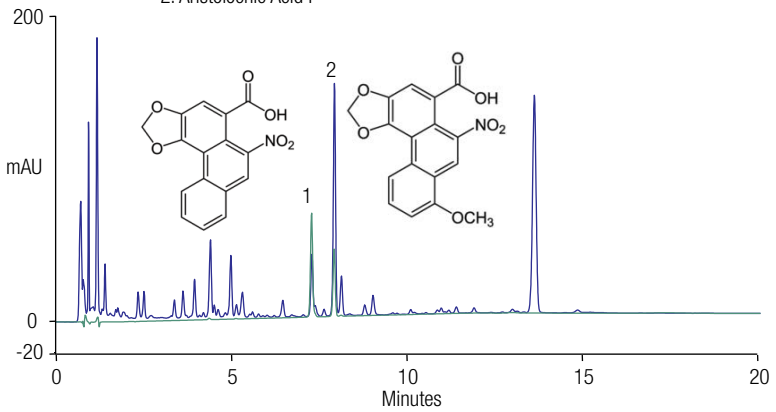


Figure 8-21. Analysis of aristolochic acid standards (green) and *Aristolochia fangchi* extract (blue) by HPLC-UV (250nm).

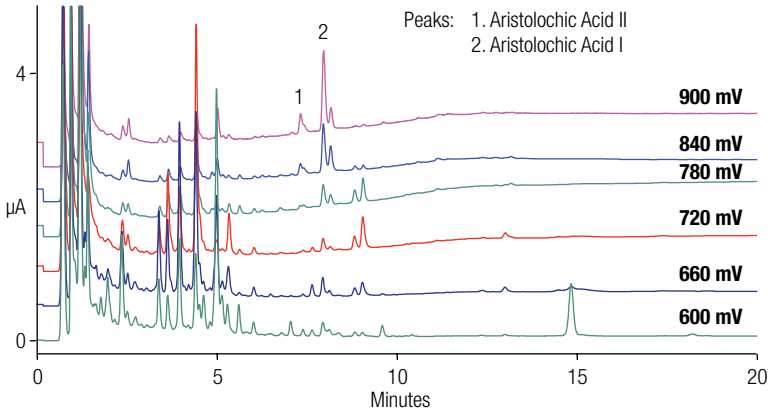
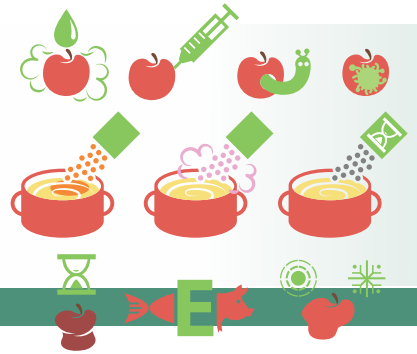


Figure 8-22. For conditions see Figure 8-21. Analysis of *Aristolochia fangchi* extract (blue) by HPLC with coulometric electrochemical array detection.



Arsenic

Growing interest around arsenic (As) determinations in fruit juices has been triggered by media claims of total arsenic concentrations above acceptable limits in apple juice products. Although the FDA has been testing and monitoring fruit juices for arsenic content for more than 20 years (and has found that total inorganic arsenic levels in juice are typically low), recently there has been heightened scrutiny of arsenic in apple juice.

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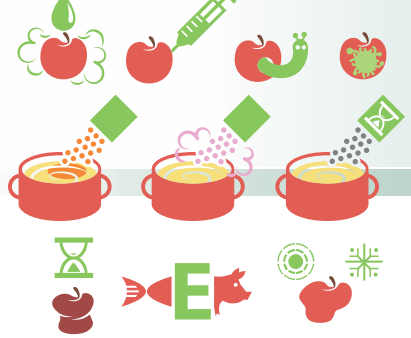


Total Inorganic Arsenic in Fruit Juice

The U.S. EPA has set the total arsenic standard for drinking water at 0.010 parts per million (ppm). However, total arsenic determinations can be misleading because inorganic arsenic compounds (arsenate As(V) and arsenite As(III)) are highly toxic, whereas organic arsenic compounds have much lower toxicity.

Technical Note 145 describes the detection and quantification of total inorganic arsenic (arsenate As(V) and arsenite As(III)) in fruit juices separated on a high-resolution 4 µm particle anion-exchange column using a high-pressure capillary IC system.

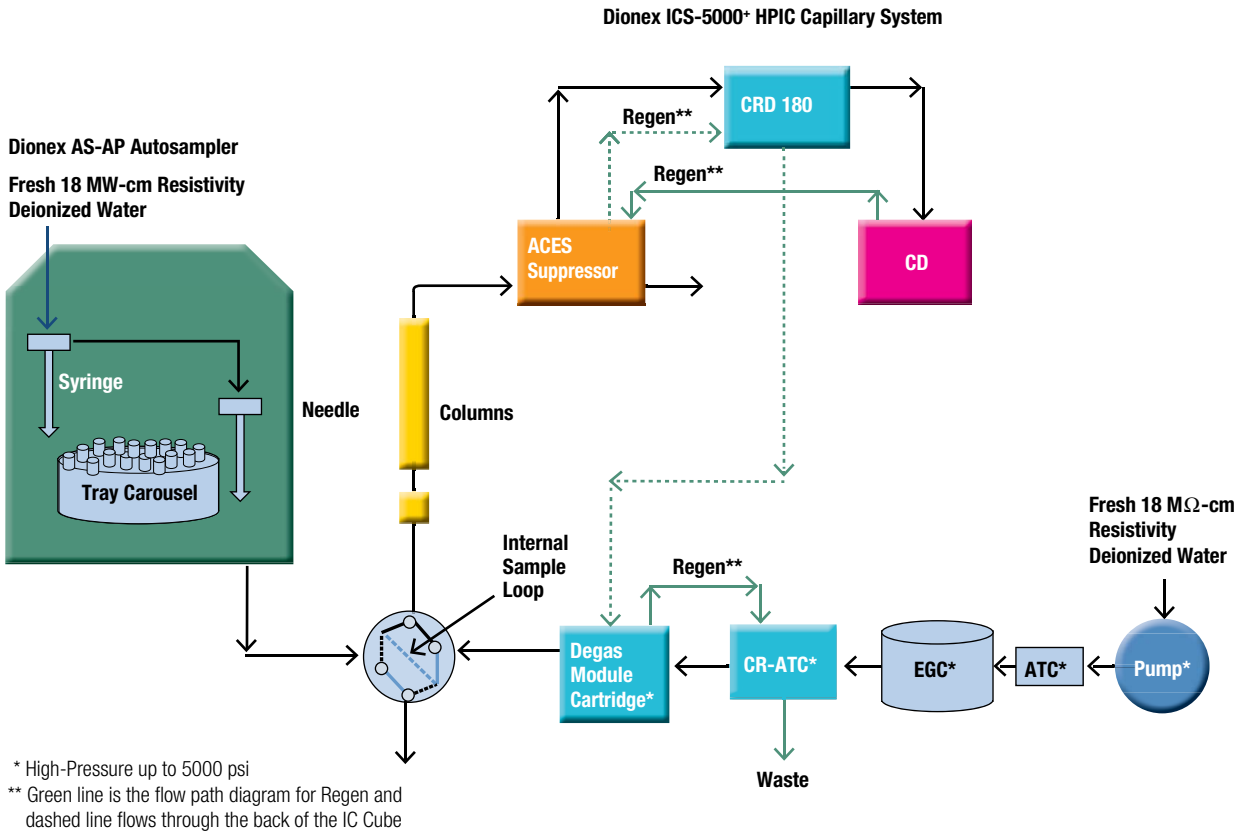


Figure 8-23. Flow diagram of the analytical system.

Download Technical Note 145: Determination of Total Inorganic Arsenic in Fruit Juice Using High-Pressure Capillary Ion Chromatography

Total Inorganic Arsenic in Fruit Juice

Instrument:	Dionex ICS-5000⁺ HPIC system
Column:	Dionex IonPac AS11-HC-4µm column, 0.4 × 250 mm
Flow:	0.015 mL/min
Column Temp.:	30 °C
IC Cube Temp.:	15 °C
Injection Volume:	0.40 µL
Eluent Source:	Thermo Scientific™ Dionex EGC-KOH cartridge (Capillary)
Gradient (KOH):	1.5–2 mM (-10–2 min), 2–8 mM (2–13 min), 8–28 mM (13–25 min), 28–35 mM (25–33 min), 35–65 mM (33–34 min), 65 mM (34–38 min)
Detection:	Suppressed conductivity, Thermo Scientific™ Dionex™ ACES™ 300 Suppressor, AutoSuppression, recycle mode
Samples:	A: Water B: 50-fold dilution of apple juice Sample 1 C: 0.2 mg/L arsenate spiked Sample B D: 0.5 mg/L arsenate spiked Sample B

Peak	mg/L	Peak	mg/L
1. Quinate	6.2	11. Malate/Succinate	73.5
2. Fluoride	1.0	12. Sulfate	1.5
3. Lactate	2.1	13. Oxalate	2.1
4. Acetate/Glycolate	3.7	14. Phosphate	3.9
5. Formate	2.6	15. Unknown	–
6. Pyruvate	0.4	16. Arsenate*	
7. Galacturonate	15.7	17. Citrate	0.5
8. Chloride	0.3	18. Isocitrate	0.2
9. Nitrate	1.1	19. trans-Aconitate	0.3
10. Glutarate	0.3	20. Unknown	–

Note that the inset is a zoomed in view of the arsenate peak.

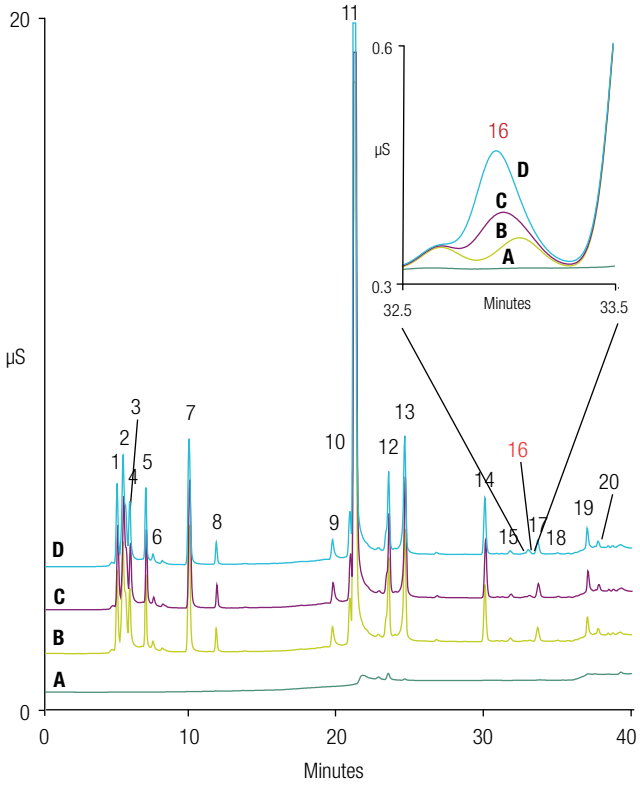


Figure 8-24. Inorganic anions, organic acids, and arsenate in a diluted apple juice sample.

Total Inorganic Arsenic in Fruit Juice

Instrument:	Dionex ICS-5000⁺ HPIC system
Column:	Dionex IonPac AS11-HC-4µm column, 0.4 × 250 mm
Flow:	0.015 mL/min
Column Temp.:	30 °C
IC Cube Temp.:	15 °C
Injection Volume:	0.40 µL
Eluent Source:	Dionex EGC-KOH cartridge (Capillary)
Gradient (KOH):	1.5–2 mM (-10–2 min), 2–8 mM (2–13 min), 8–28 mM (13–25 min), 28–35 mM (25–33 min), 35–65 mM (33–34 min), 65 mM (34–38 min)
Detection:	Suppressed conductivity, Dionex ACES 300 Suppressor, AutoSuppression, recycle mode
Samples:	A: Water B: 50-fold dilution of a grape juice sample C: 0.2 mg/L arsenate spiked Sample B D: 0.5 mg/L arsenate spiked Sample B

Peak	mg/L	Peak	mg/L
1. Quinate	14.8	10. Malate/Succinate	39.7
2. Lactate	2.1	11. Malonate/Tartrate	63.6
3. Acetate	1.9	12. Sulfate	7.8
4. Formate	1.6	13. Oxalate	1.5
5. Pyruvate	0.4	14. Phosphate	9.2
6. Galacturonate	19.1	15. Unknown	na
7. Chloride	2.4	16. Arsenate*	
8. Nitrate	1.0	17. Citrate	3.9
9. Glutarate	na	18. Isocitrate	0.7
		19. *trans*-Aconitate	na

Note that the inset is a zoomed in view of the arsenate peak.

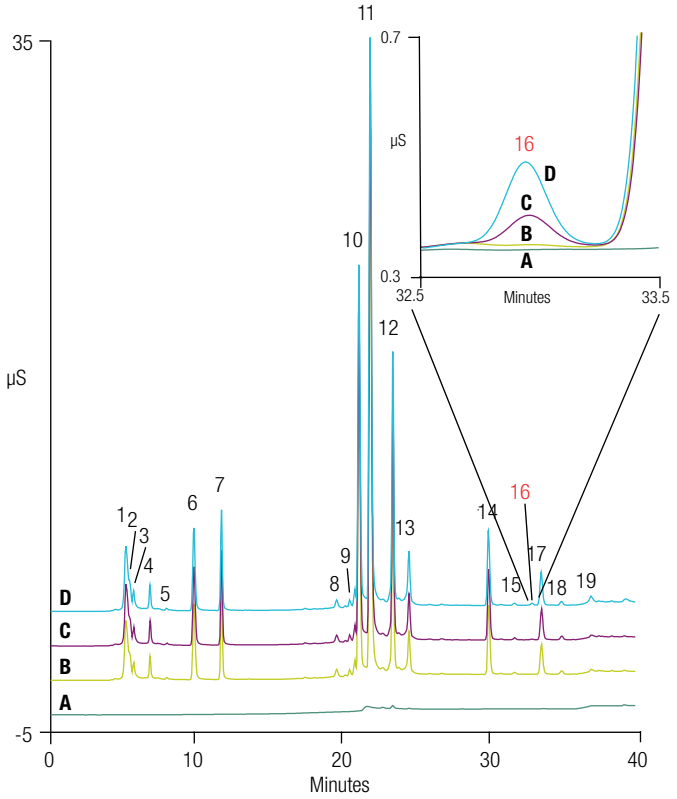


Figure 8-25. Inorganic anions, organic acids, and arsenate in a diluted grape juice sample.

Total Inorganic Arsenic in Fruit Juice

Instrument:	Dionex ICS-5000⁺ HPIC system
Column:	Dionex IonPac AS11-HC-4µm column, 0.4 × 250 mm
Flow:	0.015 mL/min
Column Temp.:	30 °C
IC Cube Temp.:	15 °C
Injection Volume:	0.40 µL
Eluent Source:	Dionex EGC-KOH cartridge (Capillary)
Gradient (KOH):	1.5–2 mM (-10–2 min), 2–8 mM (2–13 min), 8–28 mM (13–25 min), 28–35 mM (25–33 min), 35–65 mM (33–34 min), 65 mM (34–38 min)
Detection:	Suppressed conductivity, Dionex ACES 300 Suppressor, AutoSuppression, recycle mode
Samples:	A: Water B: 50-fold dilution of a mango juice sample C: 0.2 mg/L arsenate spiked into Sample B D: 0.5 mg/L arsenate spiked into Sample B

Peak	mg/L	Peak	mg/L
1. Quinate	2.3	10. Maleate	0.3
2. Lactate	2.1	11. Sulfate	0.6
3. Acetate	2.2	12. Oxalate	0.2
4. Formate	0.5	13. Phosphate	1.0
5. Galacturonate	0.6	14. Arsenate*	
6. Chloride	0.5	15. Citrate	25.4
7. Nitrate	0.7	16. Isocitrate	0.3
8. Malate/Succinate	1.1		
9. Malonate/Tartrate	0.1		

Note that the inset is a zoomed in view of the arsenate peak.

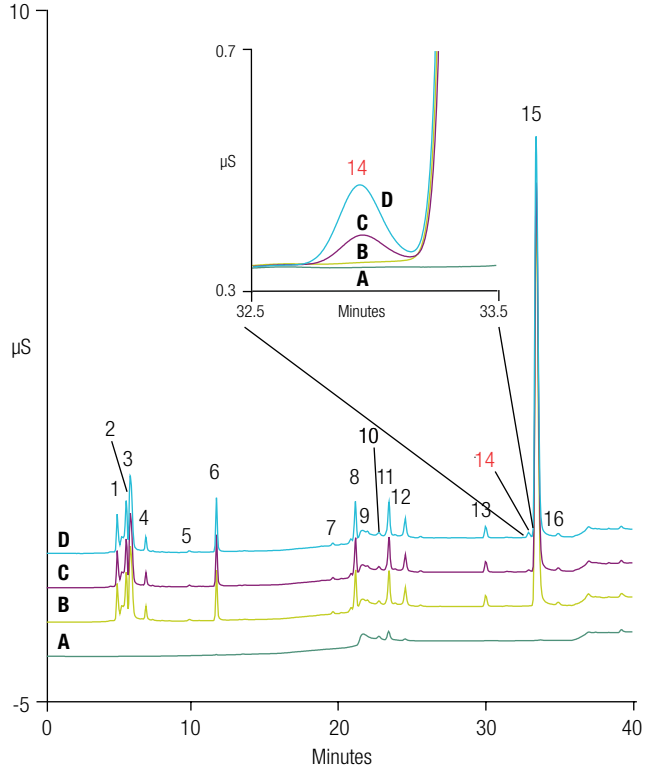


Figure 8-26. Inorganic anions, organic acids, and arsenate in a diluted mango juice sample.

Total Inorganic Arsenic in Fruit Juice

Instrument:	Dionex ICS-5000⁺ HPIC system
Column:	Dionex IonPac AS11-HC-4µm column, 0.4 × 250 mm
Flow:	0.015 mL/min
Column Temp.:	30 °C
IC Cube Temp.:	15 °C
Injection Volume:	0.40 µL
Eluent Source:	Dionex EGC-KOH cartridge (Capillary)
Gradient (KOH):	1.5–2 mM (-10–2 min), 2–8 mM (2–13 min), 8–28 mM (13–25 min), 28–35 mM (25–33 min), 35–65 mM (33–34 min), 65 mM (34–38 min)
Detection:	Suppressed conductivity, Dionex ACES 300 Suppressor, AutoSuppression, recycle mode
Samples:	A: Water B: 50-fold dilution of a cranberry cocktail juice sample C: 0.2 mg/L arsenate spiked into Sample B D: 0.5 mg/L arsenate spiked into Sample B

Peak	mg/L	Peak	mg/L
1. Quinate	38.8	10. Malate/Succinate	43.4
2. Fluoride	0.2	11. Maleate	0.8
3. Lactate	0.4	12. Sulfate	0.4
4. Acetate	0.6	13. Oxalate	–
5. Formate	0.2	14. Phosphate	0.8
6. Pyruvate	0.3	15. Unknown	na
7. Galacturonate	7.5	16. Arsenate*	
8. Chloride	0.3	17. Citrate	56.0
9. Nitrate	0.7	18. Isocitrate	0.4
		19. trans-Aconitate	0.4

Note that the inset is a zoomed in view of the arsenate peak.

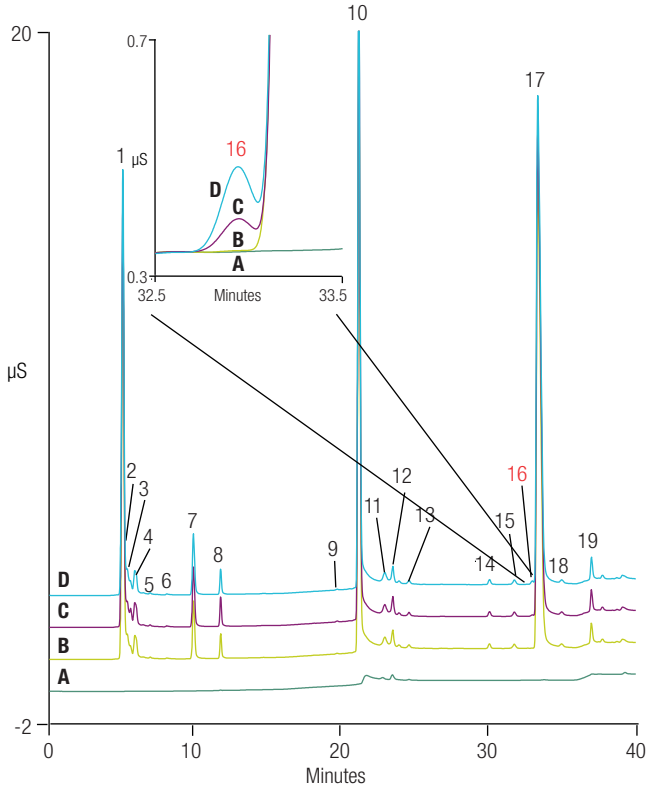


Figure 8-27. Inorganic anions, organic acids, and arsenate in a diluted cranberry cocktail juice.

Total Inorganic Arsenic in Fruit Juice

Instrument:	Dionex ICS-5000⁺ HPIC system
Column:	Dionex IonPac AS11-HC-4µm column, 0.4 × 250 mm
Flow:	0.015 mL/min
Column Temp.:	30 °C
IC Cube Temp.:	15 °C
Injection Volume:	0.40 µL
Eluent Source:	Dionex EGC-KOH cartridge (Capillary)
Gradient (KOH):	1.5–2 mM (-10–2 min), 2–8 mM (2–13 min), 8–28 mM (13–25 min), 28–35 mM (25–33 min), 35–65 mM (33–34 min), 65 mM (34–38 min)
Detection:	Suppressed conductivity, Dionex ACES 300 Suppressor, AutoSuppression, recycle mode
Samples:	A: Water B: 1 mg/L arsenate in water C: 50-fold dilution of apple juice Sample 1 D: 0.50 mg/L arsenate spiked Sample C E: 50-fold dilution of apple juice Sample 2 F: 50-fold dilution of apple juice Sample 3

Note that the inset is a zoomed in view of the arsenate peak.

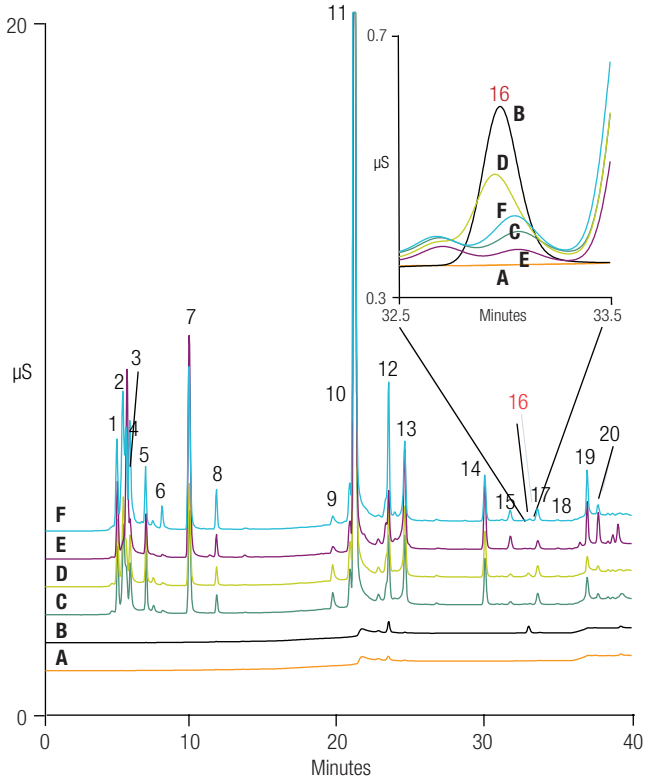
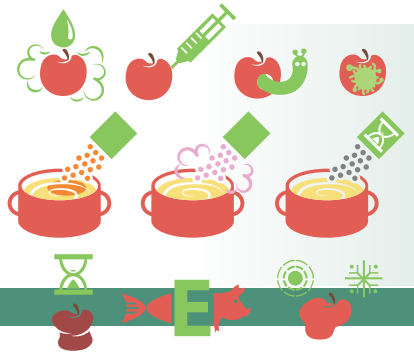
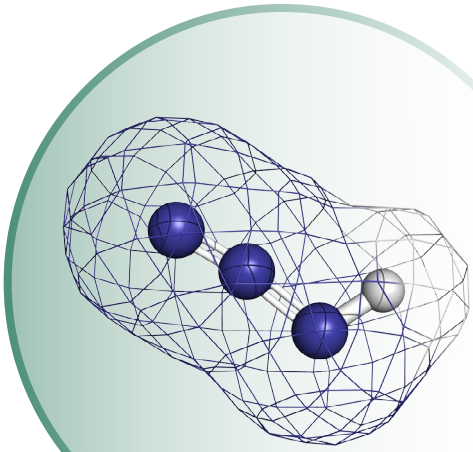


Figure 8-28. Inorganic anions, organic acids, and arsenate in diluted apple juice samples.





Structure of hydrazoic acid

Azide

Sodium azide, a salt of hydrazoic acid, is a white crystalline solid that is highly toxic when ingested or inhaled. The salt readily dissolves in water to yield the azide anion(N_3^-). Contact with water or acid causes release of hydrazoic acid (HN_3), a gas with a sharp, disagreeable odor that is considerably more toxic than the salt.

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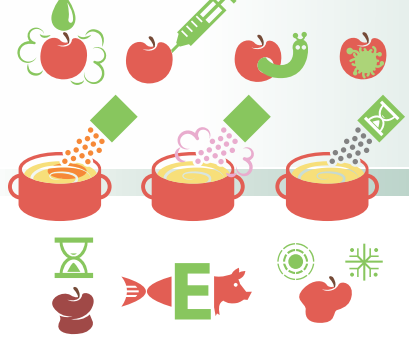

Azide

Azide anions prevent the cells of the body from using oxygen, inhibiting the function of cytochrome oxidase by binding irreversibly to the heme cofactor. Fatal doses occur with exposures of 700 mg (10 mg/kg), but exposure to smaller doses can cause eye and skin irritation, headache, nausea, shortness of breath, dizziness, blurred vision, low blood pressure, or kidney damage.

Sodium azide is used in automobile airbags, as a chemical preservative in hospitals and laboratories, in agriculture for pest control, in pharmaceutical manufacturing, and in detonators and other explosives. Azide is also of interest to forensic investigators. Several people were poisoned in Japan in 1998 when azide was added into tea and orange juice. Ion chromatography was a key tool in diagnosing the cause of this poisoning.

Application Note 172 describes how to routinely monitor the azide anion in aqueous samples including water, food products, bodily fluids, and biological buffers by using a Reagent-Free IC system.

Column:	Dionex IonPac AG15, AS15, 4 mm	Peaks:	1. Fluoride	0.5 mg/L
Flow:	1.2 mL/min		2. Chloride	0.6
Temperature:	30 °C		3. Oxalate	1.6
Injection Volume:	25 µL		4. Sulfate	1.7
Eluent:	42 mM KOH		5. Azide	10.2
Detection:	Suppressed conductivity, Dionex ASRS ULTRA II, recycle mode			

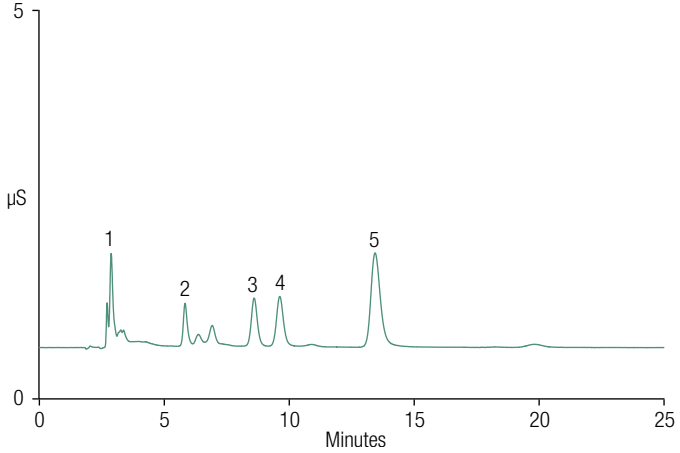

Figure 8-29. Determination of 10 mg/L azide spiked into 10-fold diluted green tea.

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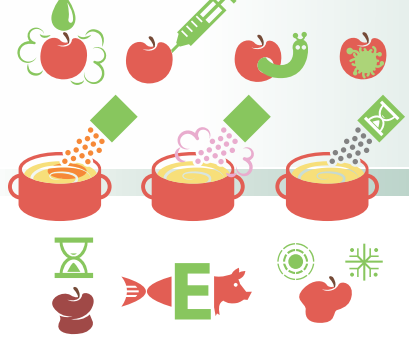
Download Application Note 172: Determination of Azide in Aqueous Samples by Ion Chromatography with Suppressed Conductivity Detection



Azide

Column:	Dionex IonPac AG15, AS15, 4 mm	Peaks:	1. Fluoride	4.2	mg/L
Flow:	1.2 mL/min		2. Sulfate	16.2	
Temperature:	30 °C		3. Fumarate	74.2	
Injection Volume:	25 µL		4. Azide	10.2	
Eluent:	42 mM KOH		5. Phosphate	31.0	
Detection:	Suppressed conductivity Dionex ASRS ULTRA II suppressor, recycle mode				

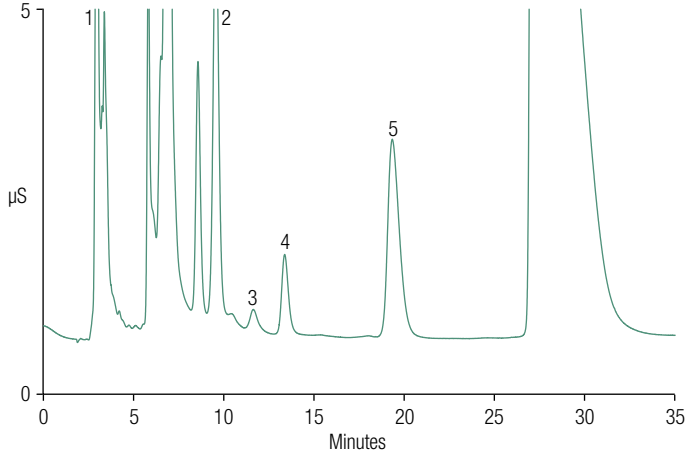


Figure 8-30. Determination of 10 mg/L azide spiked into 10-fold diluted orange juice.

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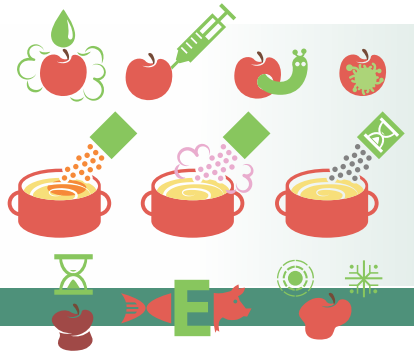

Spoiled cheese

Biogenic Amines

Biogenic amines are organic bases commonly present in living organisms, where they are responsible for many essential functions. Biogenic amines (BAs) in food and meat products are related to both food spoilage and food safety.

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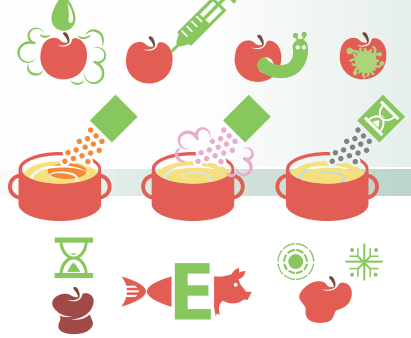

Biogenic Amines

Determination of biogenic amines (BA) (cadaverine, putrescine, spermidine, histamine, phenyethylamine, agmatine, and tyramine) in fresh and processed food is of great interest, not only because of their toxicity, but also because of their use as spoilage indicators.

Various HPLC methods have been developed for determination of BAs in foods, but due to lack of suitable chromophoric or fluorophoric groups, almost all of the proposed methods require pre- or postcolumn derivatization to provide sufficient sensitivity.

Such limitations can be overcome through the use of a novel cation-exchange selectivity column coupled with conductivity and MS detection in series.

Columns:	Dionex IonPac CG17 (2 × 50 mm) and IonPac CS17 (2 × 250 mm)
Flow:	0.38 mL/min
Temperature:	40 °C
Injection Volume:	5 µL
Eluent:	MSA from EG50
Gradient:	7 min isocratic at 3 mmol/L MSA prior to injection, then 6 min isocratic at 3 mmol/L, then in 20 min to 30 mmol/L for additional 14 min
Suppressor:	Dionex CSRS ULTRA II suppressor (2 mm), Current: 50 mA,
Detection:	1) Conductivity 2) MSQ, ESI+, needle voltage: 3.0 kV; probe temperature: 400 °C; cone voltage: 50 V; dwell time: 0.2 s

Peaks:		
	1. Putrescine	89 *m/z*
	2. Cadaverine	103
	3. Histamine	112
	4. Agmatine	131
	5. Phenethylamine	122
	6. Spermidine	146

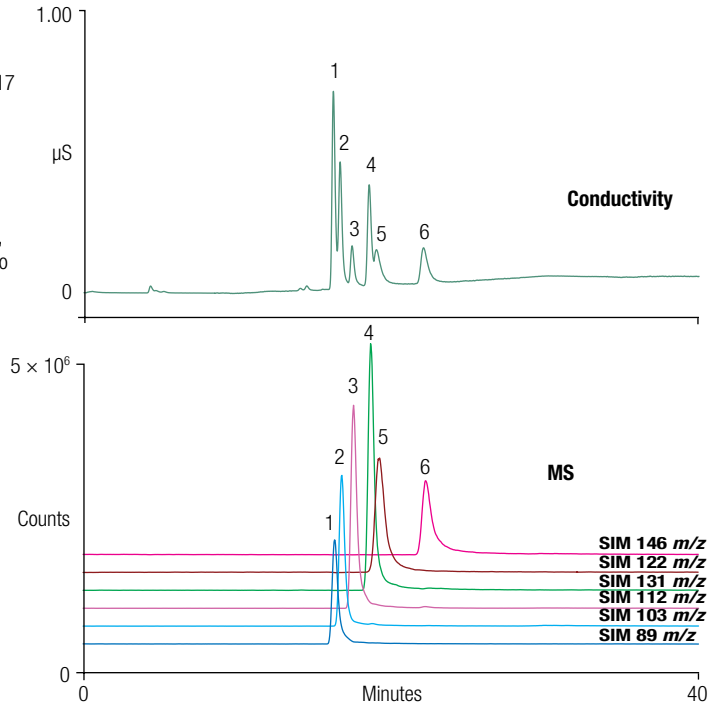

Figure 8-31. Cation-exchange chromatographic separation of biogenic amines standard solution (5 mg/L each) using gradient elution with suppressed conductivity and MS detection.

Biogenic Amines in Meat Products

Columns:	Dionex IonPac CG17 (2 × 50 mm) and IonPac CS17 (2 × 250 mm)
Flow:	0.38 mL/min
Temperature:	40 °C
Injection Volume:	5 µL
Eluent:	MSA from EG50
Gradient:	7 min isocratic at 3 mmol/L MSA prior to injection, then 6 min isocratic at 3 mmol/L, then in 20 min to 30 mmol/L for additional 14 min
Suppressor:	Dionex CSRS ULTRA II suppressor (2 mm), Current: 50 mA, external water mode
Detection:	1. Conductivity 2. MSQ, ESI+, needle voltage: 3.0 kV; probe temperature: 400 °C; cone voltage: 50 V; dwell time: 0.2 s

Peaks:		
1.	Putrescine	89 *m/z*
2.	Cadaverine	103
3.	Histamine	112
4.	Agmatine	131
5.	Phenethylamine	122
6.	Spermidine	146

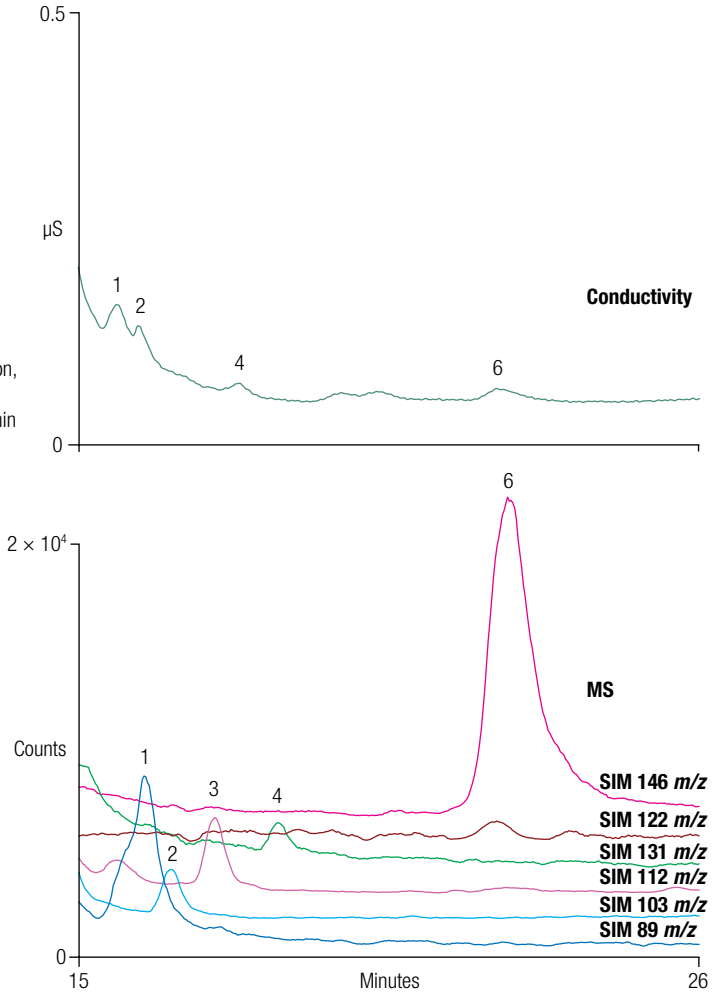

Figure 8-32. Amounts of biogenic amines in raw or cooked ham are generally much lower than those in fermented sausage and far from any toxic level. Using conductivity detection a small amount of agmatine (Peak 4) was observed in cooked ham and this was confirmed by MS.

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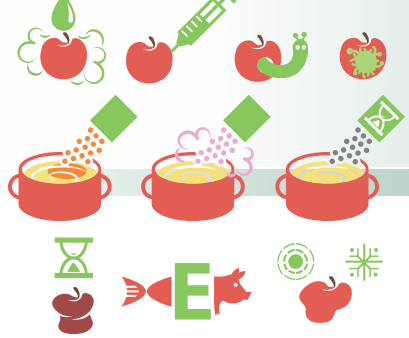

Biogenic Amines in Spoiled Products

Another IC approach determining biogenic amines is a cation-exchange separation followed by electrochemical detection using integrated pulsed amperometry (IPAD) on a gold working electrode. IPAD can also be used a second detector after suppressed conductivity. A few biogenic amines have a good UV chromophore (e.g. tyramine) and can be detected in that manner after a cation-exchange separation. UV detection can also be used in combination with suppressed conductivity or IPAD detection.

Column: Dionex IonPac CG18, CS18, 2 mm
Flow: 0.30 mL/min
Temperature: 40 °C
Injection Volume: 5 µL
Eluent: Methanesulfonic acid: 3 mM from 0–6 min, 3–10 mM from 6–10 min, 10–15 min from 10–22 min, 15 mM from 22–28 min, 15–30 mM from 28-35 min, 45 mM from 35.1–40 min
Eluent Source: EGC II MSA
Detection: A) Integrated pulsed amperometric detection
B) UV absorbance at 276 nm
Postcolumn Reagent: 0.1 M NaOH
PCR Flow Rate: 0.24 mL/min

Peaks:		A	B	
	1. Tyramine	1157	1139	mg/kg

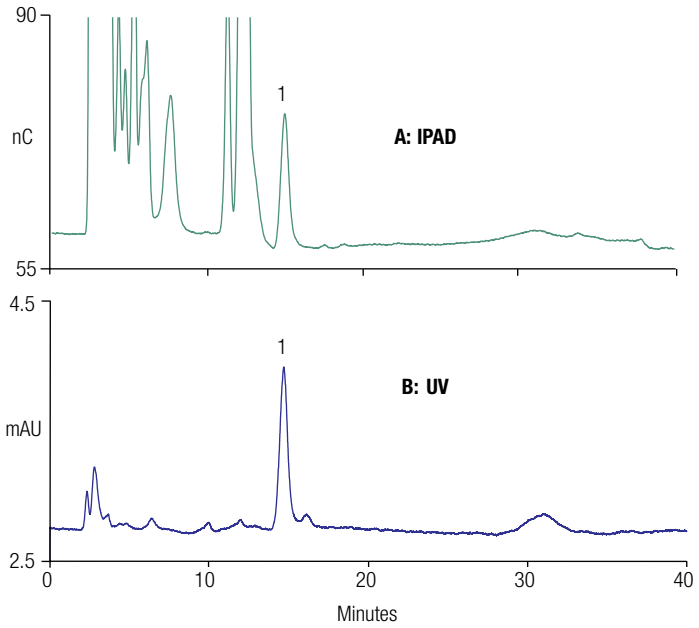

Figure 8-33. Determination of biogenic amines in spoiled Swiss cheese by (A) IPAD and (B) UV detection.

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Biogenic Amines in Spoiled Products

Column:	Dionex IonPac CG18, CS18, 2 mm
Flow:	0.30 mL/min
Temperature:	40 °C
Injection Volume:	5 µL
Eluent:	Methanesulfonic acid: 3 mM from 0–6 min, 3–10 mM from 6–10 min, 10–15 min from 10–22 min, 15 mM from 22–28 min, 15–30 mM from 28-35 min, 45 mM from 35.1–40 min
Eluent Source:	EGC II MSA
Detection:	Suppressed conductivity, Dionex CSRS ULTRA II suppressor, 2 mm, AutoSuppression, external water mode

Peaks:		A	B	
	1. Putrescine	0.65	9.5	mg/kg
	2. Cadaverine	—	3.1	
	3. Histamine	—	1.6	
	4. Agmatine	8.2	6.9	
	5. Spermidine	7.6	14.3	
	6. Spermine	46.6	32.1	

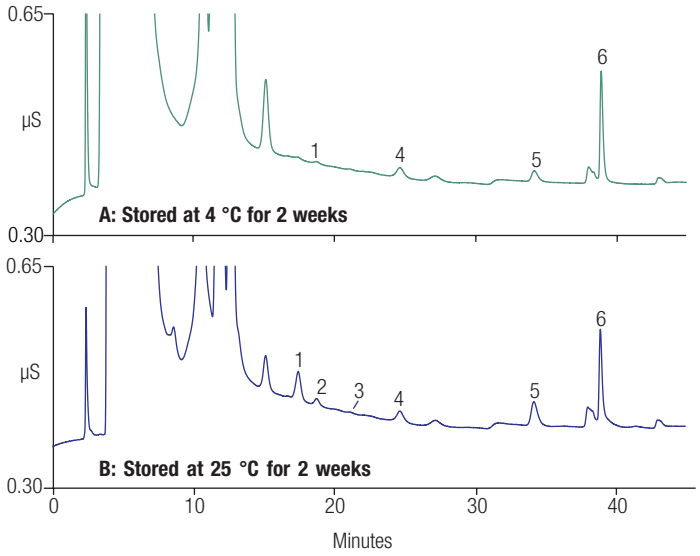
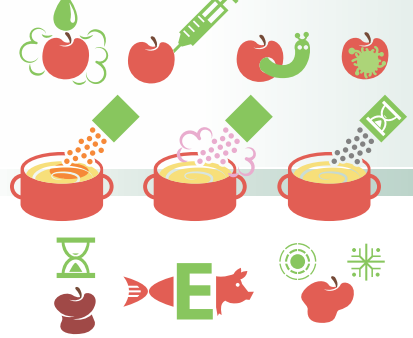


Figure 8-34. Determination of biogenic amines in spoiled sausage by IC with suppressed conductivity detection.

Download Application Note 183: Determination of Biogenic Amines in Fermented and Non-Fermented Foods Using Ion Chromatography with Suppressed Conductivity and Integrated Pulsed Amperometric Detections



Biogenic Amines in Alcoholic Beverages

Malolactic fermentation or the action of yeasts in primary fermentation has been associated with the production of biogenic amines such as tyramine, putrescine, cadaverine, histamine, and phenylethylamine in wine samples. Histamine can produce headaches, flushing of the face and neck, and hypotension, whereas some aromatic amines, such as tyramine and phenylethylamine, can cause migraines and hypertension. The concentration and content of biogenic amines in wines are variable depending on the storage time and conditions, quality of raw materials, and possible microbial contamination during the winemaking process.

Putrescine, agmatine, spermidine, and spermine are considered natural beer constituents that primarily originate from malt. The presence of tyramine, cadaverine, and histamine, however, has been associated with the activities of contaminating lactic acid bacteria during the brewing process.

Application Note 182 describes a straightforward and direct way to measure biogenic amines in alcoholic beverages using ion chromatography with suppressed conductivity and integrated pulsed amperometric detection.

Column:	Dionex IonPac CG18, CS18, 2 mm
Flow:	0.30 mL/min
Temperature:	40 °C
Injection Volume:	5 µL
Eluent:	Methanesulfonic acid: 3 mM from 0–6 min, 3–10 mM from 6–10 min, 10–15 mM from 10–22 min,15 mM from 22–28 min, 15–30 mM from 28–35 min, 30–45 mM from 35.1–45 min
Eluent Source:	EGC II MSA
Detection:	A. Integrated Pulsed Amperometric Detection B. Absorbance, 276 nm
Postcolumn Reagent:	0.1 M NaOH
PCR Flow Rate:	0.24 mL/min

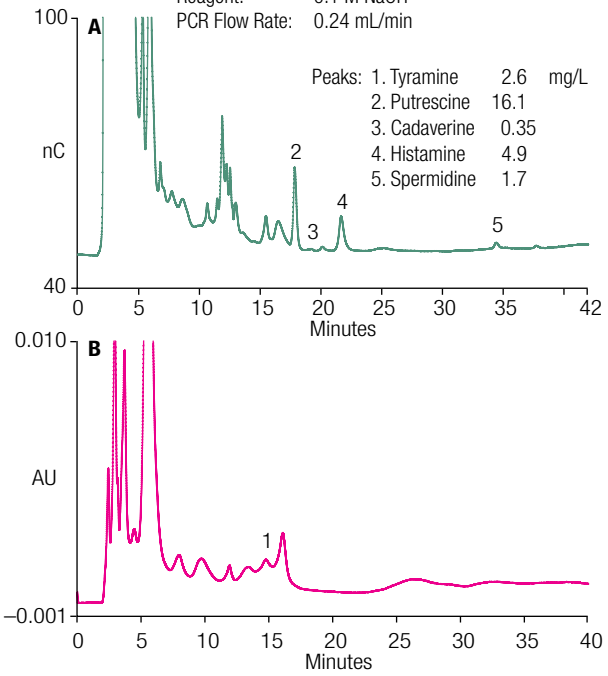
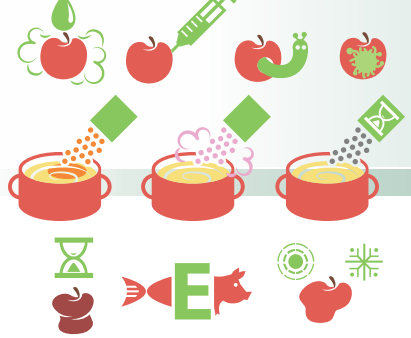


Figure 8-35. Determination of biogenic amines in a California Cabernet Sauvignon by (A) IPAD and (B) UV absorbance detection.

Download Application Note 182: Determination of Biogenic Amines in Alcoholic Beverages by Ion Chromatography with Suppressed Conductivity and Integrated Pulsed Amperometric Detections



Biogenic Amines in Alcoholic Beverages

Column: Dionex IonPac CG18, CS18, 2 mm
Flow: 0.30 mL/min
Temperature: 40 °C
Injection Volume: 5 µL
Eluent: Methanesulfonic acid: 3 mM from 0–6 min, 3–10 mM from 6–10 min,10–15 mM from 10–22 min, 15 mM from 22–28 min, 15–30 mM from 28–35 min, 30–45 mM from 35.1–42 min
Eluent Source: EGC II MSA
Detection: Suppressed conductivity, Dionex CSRS ULTRA II suppressor, 2 mm, AutoSuppression external water mode

Peaks:		
	1. Putrescine	6.6 mg/L (ppm)
	2. Cadaverine	0.67
	3. Histamine	0.60
	4. Agmatine	7.70
	5. Spermidine	1.2
	6. Spermine	0.73

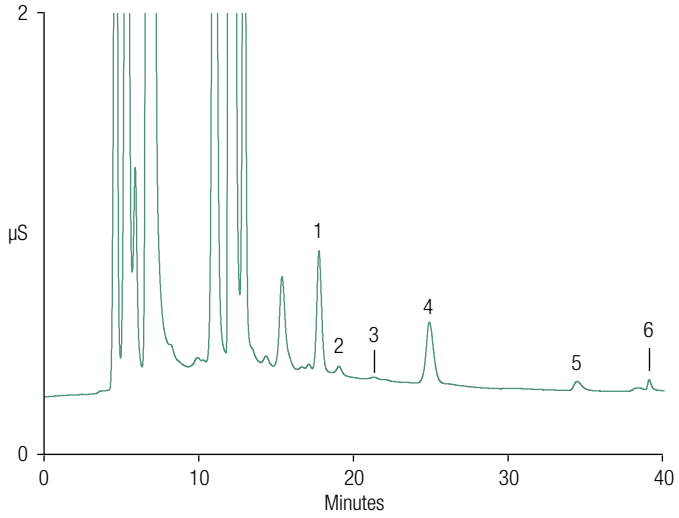


Figure 8-36. Determination of biogenic amines in wheat beer using suppressed conductivity detection.

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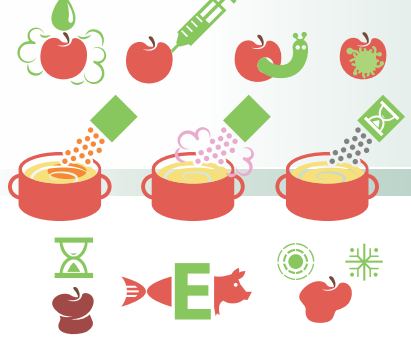

Biogenic Amines in Alcoholic Beverages

Table 8-5. Biogenic amine concentrations in stored alcoholic beverages determined by suppressed conductivity detection and IPAD.

Suppressed Conductivity Detection												
Sample	Putrescine		Cadaverine		Histamine		Agmatine		Spermidine		Spermine	
	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)
Wheat Beer #1[a]	6.4±0.0	96.0	0.28±0.02	91.4	0.54±0.02	95.4	9.1±0.0	102.3	0.45±0.01	101.0	0.47±0.02	113.0
Wheat Beer #2[b]	6.6±0.0	95.8	0.67±0.00	88.5	0.60±0.01	99.0	7.7±0.0	102.4	1.2±0.0	104.0	0.73±0.01	117.5
Lager Beerc	3.0±0.0	101.2	<DL[d]	—	0.72±0.03	98.2	14.9±0.1	104.8	0.14±0.01	104.3	0.33±0.02	—
California Cabernet Sauvignona	19.4±0.1	97.6	0.79±0.00	103.1	5.51±0.06	103.7	0.37±0.00	89.3	1.9±0.0	101.6	0.19±0.01	121.9
Australian Cabernet Sauvignon[b]	7.1±0.1	95.8	0.53±0.01	88.5	0.84±0.03	99.0	0.23±0.02	95.8	1.4±0.0	104.0	0.21±0.02	100.0
Pinot Grigioc	1.7±0.0	103.5	<DL	—	<DL	—	<DL	—	<DL	—	<DL	—
IPAD (post-suppression)												
Sample	Putrescine		Cadaverine		Histamine		Agmatine		Spermidine		Spermine	
	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)	Amount Found (mg/L)	Recov. (%)
Wheat Beer #1	6.2±0.1	96.0	<DL	—	<DL	—	8.7±0.2	94.0	0.42±0.00	100.6	0.48±0.01	97.3
Wheat Beer #2	5.8±0.1	95.6	<DL	—	<DL	—	7.2±0.1	87.2	1.2±0.0	95.4	0.67±0.03	110.8
Lager Beer	3.0±0.0	94.6	<DL	—	<DL	—	14.5±0.1	93.7	<DL	—	<DL	—
California Cabernet Sauvignon	22.1±0.4	106.5	<DL	—	5.4±0.2	99.3	<DL	—	2.0±0.1	100.6	<DL	—
Australian Cabernet Sauvignon	6.9±0.3	103.6	<DL	—	0.67±0.04	98.1	<DL	—	1.5±0.0	104.9	<DL	—
Pinot Grigio	1.5±0.1	100.7	<DL	—	<DL	—	<DL	—	<DL	—	<DL	—

Stored at 4 °C for [a]3 weeks, [b]1 week, [c]2 weeks.
[d]<DL = less than the detection limit.

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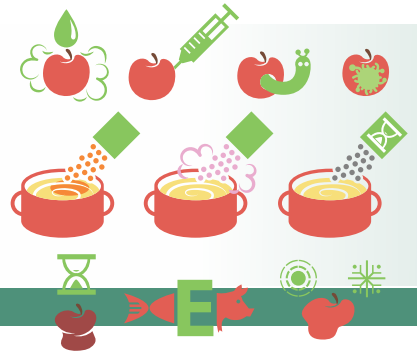

Bisphenol A

Bisphenol A (BPA) is widely used in high production volume manufacturing of polycarbonate plastics (e.g., food containers and plastic bottles) and epoxy resins. Current studies evaluating the impact of BPA on health and the environment have not reported conclusive results, however, actions have been taken proactively to protect sensitive populations.

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Bisphenol A

Bisphenol A by LC with MS Detection

Canada proposed banning BPA to reduce the exposure for newborns and infants in 2009, and the U.S. Environmental Protection Agency (EPA) recently added BPA to its list of target chemicals for possible regulation. Octylphenol (OP) and nonylphenol (NP) are the degradation products of widely used nonionic surfactants: alkylphenol ethoxylates. The estrogenic and toxic effects of OP and NP have been well studied and reported. Recent reports show NP being detected in food and food wraps, posing more concerns for food safety and food packaging.

The application described here is a high-throughput LC-MS method for simultaneous quantitative analysis of BPA, *4-t-OP, 4-n-OP,* and *4-n-NP.*

System:	UltiMate 3000 HPLC
Column:	Acclaim PA2 RSLC column, 2.1 × 50 mm, 2.2 µm
Flow:	0.5 mL/min
Temperature:	30 °C
Injection Volume:	100 µL
Mobile Phase:	Methanol and DI water gradient: 75% to 95% methanol from 0.1 to 1.3 min, hold for 1.1 min and return to initial condition, and equilibrate for 1 min
Analyte:	BPA 1 ppb and phenols 2 ppb in bottled water sample

Mass Spectrometric Conditions

System:	MSQ Plus single quadrupole mass spectrometer
Interface:	APCI
Probe Temp:	500 °C
Nebulizer Gas:	Nitrogen at 55 psi
Corona Current:	50 µA
Detection Mode:	Negative SIM
	Cone voltage set at 65 V for all SIM scans
	BPA: 227 *m/z*
	BPA-IS: 241 *m/z*
	4-t-OP: 205 *m/z*
	4-n-OP: 205 *m/z*
	4-n-NP: 219 *m/z*

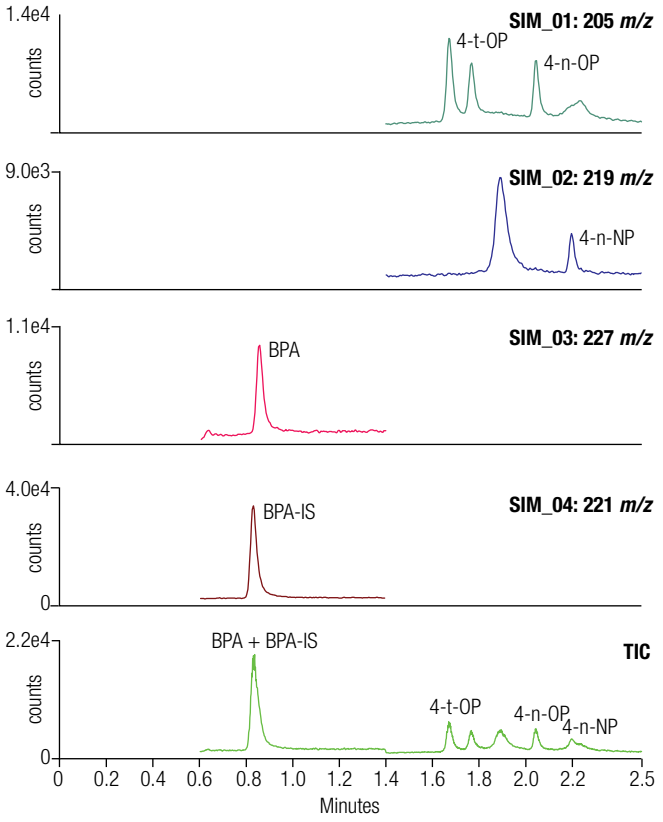
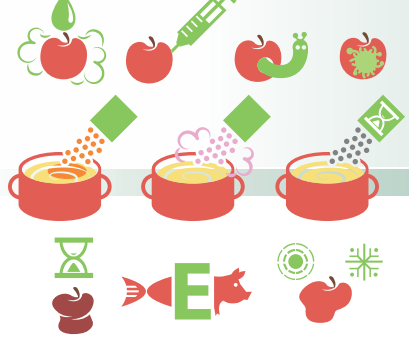


Figure 8-37. SIM and TIC chromatograms of a bottled water sample spiked with 1 ppb BPA and 2 ppb phenols.

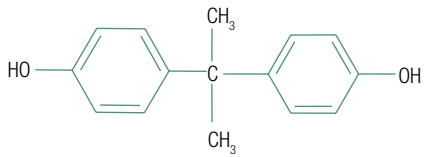


Bisphenol A

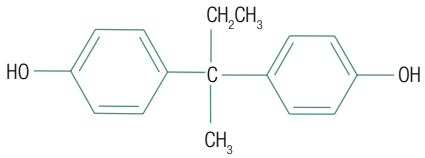
Bisphenol A by HPLC with Electrochemical Array Detection

Xeonestrogens are a diverse group of compounds found in the envirnonment that mimic the effects of endogenous estrogens. Xenoestrogens bio-accumulate in higher organisms that form part of the human diet. Evidence suggests that exposure to xenoestrogens may be associated with increased incidence of cancer. Bisphenols A and B are monomers used in the production of epoxy resins and plastics that are used in food and drink packaging, as coatings in metal cans and in microwave susceptors (used to crispen food).

Presented here is a general method using gradient HPLC and electrochemical array detection capable of measuring Bisphenol A and B, a number of phytoestrogens and diethylstibestrol (DES). The method can be applied to foods, and has sufficient sensitivity and selectivity to measure analytes in plasma.



Bisphenol A



Bisphenol B

Figure 8-38. Chemical structures of Bisphenols A and B.

Column:	C18 (3 × 150; 3 µm)
Flow:	0.6 mL/min
Column Temp.:	Ambient
Injection Volume:	20 µL
Mobile Phase:	A: 50 mM Sodium acetate (pH 4.8); methanol (80:20 v/v)
	B: 50 mM Sodium acetate (pH 4.8); methanol; acetonitrile (40:40:20 v/v/v)
Detector:	CoulArray
Applied potentials (mV):	+380, +400, +440, +500, +560, +620, +680, +760

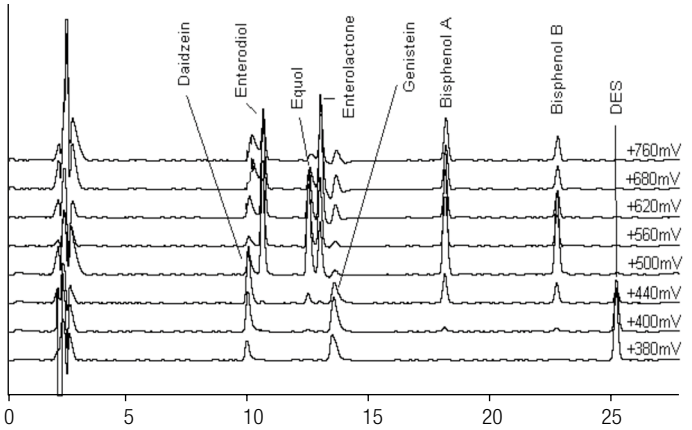
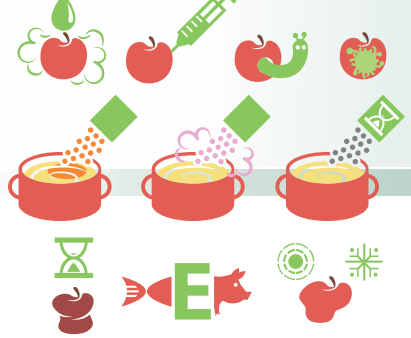


Figure 8-39. Gradient chromatogram of bisphenols, phytoestrogens, and DES standards.



Bisphenol A

Bisphenol-A Diglycidyl Ethers

BADGE is a widely-used epoxy monomer derived from bisphenol-A. Because epoxies are used in food-contact applications, the residues of this group of substances are of concern to public health officials. Dionex Accelerated Solvent Extraction technology rapidly extracts the residues, then the RSLC system rapidly quantifies them.

Chromatograms:
A. Standards, 16.7 µg/mL in acetonitrile
B. Tuna canned in water, control
C. Tuna canned in water, spiked 20 mg/kg
D. Tuna canned in oil, control
E. Tuna canned in oil, spiked 20 mg/kg

Pump:	UltiMate HPG-3200 RS
Column:	Acclaim 120 C18 RSLC, 2.2 µm, 2.1 × 50 mm
Flow:	0.49 mL/min
Temperature:	TCC-3000 RS thermostat at 30 °C
Injection:	WPS-3000 RS sampler at 0.7 µL
Mobile Phases:	A: Methanol B: Water

Gradient:

	–4.5	0.0	0.1	1.8	3.5
%A	50	50	50	80	80
%B	50	50	50	20	20

sample loop bypass at 0.2 min

Detector:	DAD-3000 RS, UV 277 and 228 nm
Sample Prep:	ASE extraction of 5 g sample with 60 mL of 4:1 hexane:acetone at 100 °C. Dry over anh. Na_2SO_4, then evaporate to ~ 10 mL. Extract with 3 × 2 mL of acetonitrile

Peaks:
1. BADGE-2H_2O
2. Bisphenol-A
3. BADGE-H_2O
4. BADGE-H_2O-HCl
5. BADGE
6. BADGE-HCl
7. BADGE-2HCl

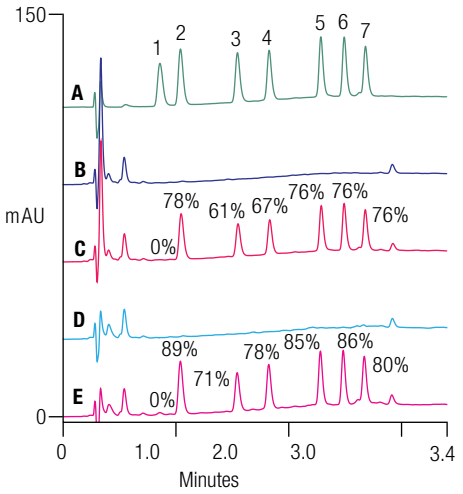


Figure 8-40. Recovery of bisphenol-A diglycidyl ether (BADGE) and related impurities from canned tuna using the Acclaim 120 C18 RSLC column.

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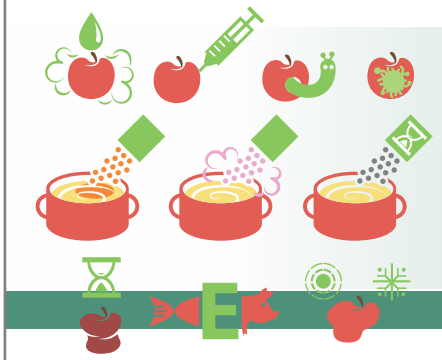

Carbamate Pesticides

The *N*-methylcarbamates and the *N*-methylcarbamoximes are among the most widely used pesticides in agriculture. Because these pesticides may create health problems – including issues impacting the central nervous and reproductive systems – concerns over the presence of carbamate residues in water, crops, and food products have promoted increased awareness and testing for these compounds.

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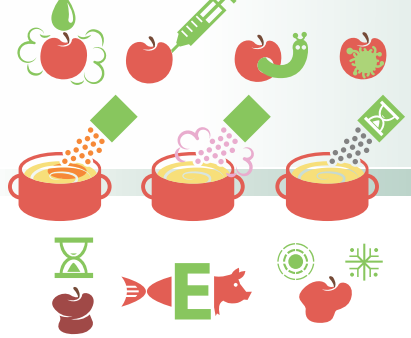

Carbamate Pesticides in Rice

For the detection of carbamate residues in food matrices, sample preparation is key for a sensitive determination. The work shown here uses a two-step sample preparation method that first uses a salting-out extraction to extract the target analytes, then a dispersive solid-phase extraction (dSPE) to remove sugars, lipids, organic acids, sterols, proteins, and pigments. Similar methods are now available, such as AOAC 2007.01 Method11 by the Association of Official Analytical Chemists (AOAC) in the United States, and the European equivalent, EN 15662.

Fluorescence Detection

The separation is performed on an Acclaim Carbamate column with detection by a FLD-3400RS fluorescence detector. The chromatography method is based on a reversed-phase separation of the carbamates with subsequent derivatization by o-Phthalaldehyde (OPA) followed by fluorescence detection..

Guard Column:	Acclaim Carbamate, 3.0 × 10 mm, 3 µm
Analytical Column:	Acclaim Carbamate, 3.0 × 150 mm, 3 µm
Flow:	0.9 mL/min
Column Temperature:	50 °C
Injection Volume:	50 µL
Mobile Phase:	Methanol - H_2O, in Gradient: Methanol, -4.0–0.0 min, 14%; 2.0 min, 20%; 8.0 min, 40%; 13.6–16 min, 70%
Post Column Reagent 1:	0.2% NaOH, first reaction coil at 100 °C
Post Column Reagent 2:	OPA regent, second reaction coil at room temperature
Flow Rate of Reagent 1 and 2:	0.3 mL/min
Fluorescence Detection:	Excitation, 330 nm; emission, 465 nm
Chromatograms:	(A) without dSPE; and (B) with dSPE using PSA (Primary secondary amine Bonded Silica)

Peaks:
1. Aldicarb sulfoxide
2. Aldicarb sulfone
3. Oxamyl
4. Methomyl
5. 3-Hydroxy carbofuran
6. Aldicarb
7. Propoxur
8. Carbofuran
9. Carbaryl
10. 1-Naphthol
11. Methiocarb

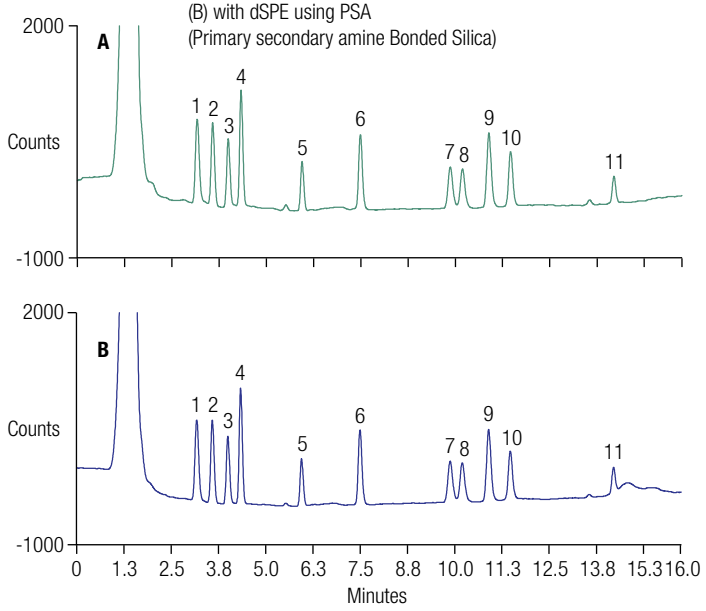

Figure 8-41. Chromatograms of extracts of carbamate standard- spiked rice samples (2 µg/L each) after acetonitrile and salt-out extractions (A) without and (B) with SPE using PSA.

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Carbamate Pesticides in Corn and Potato

Fluorescence Detection

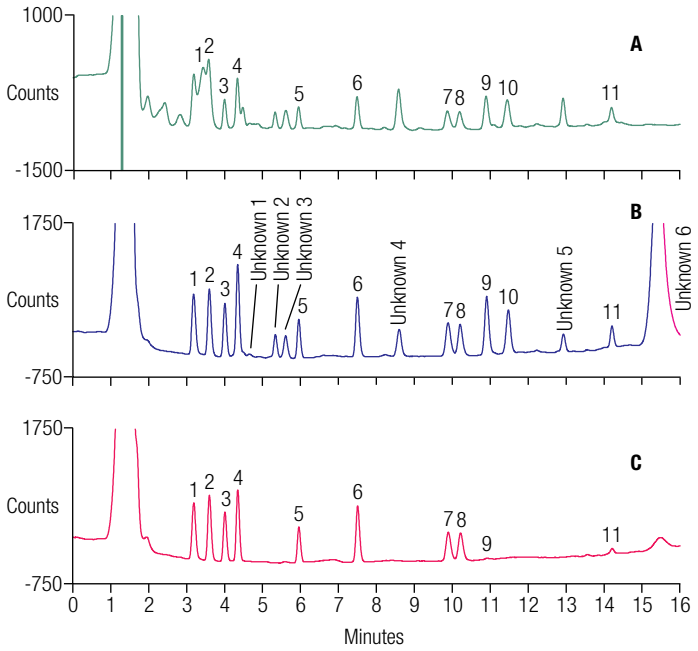

Figure 8-42. Chromatograms of extracts of carbamate standard- spiked corn samples (2 µg/L each) after acetonitrile and salt-out extractions (A) without and with dSPE using (B) PSA and (C) activated carbon. For conditions and name key see Figure 8-35.

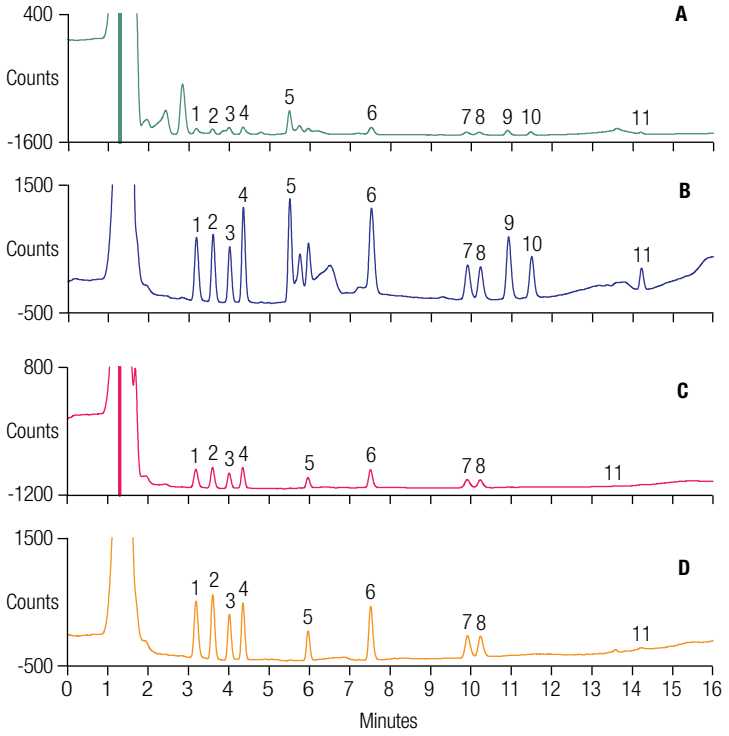

Figure 8-43. Chromatograms of extracts of carbamate standard- spiked potato samples (2 µg/L each) after acetonitrile and salt-out extractions (A) without and with dSPE using (B) PSA, (C) activated carbon, and (D) mixture of PSA and activated carbon (1:1, w/w). For conditions see Figure 8-35.

Carbamate Pesticides

MS Detection

Carbamate pesticides can be separated using a 2.1 × 150 mm Acclaim Carbamate column and detected using MS. This method has been successfully applied to the determination of carbamates in various types of water samples.

Chromatographic Conditions

System: UltiMate 3000 HPLC system
Column: Acclaim Carbamate (2.1 × 150 mm, 3 µm)

Flow: 300 µL/min
Injection Volume: 20 µL
Mobile Phase: A) Methanol
B) 1.0 mM Ammonium formate
C) Water

Time (min)	A%	B%	C%
–4.0	10	5	85
0.0	10	5	85
2.0	10	5	85
15.0	65	5	30
15.1	90	5	5
20.0	90	5	5

Detector: MSQ Plus single quadrupole mass spectrometer

Mass Spectrometric Conditions

Ionization interface: Electrospray Ionization (ESI) positive mode
Detection mode: Selected Ion Monitoring (SIM)

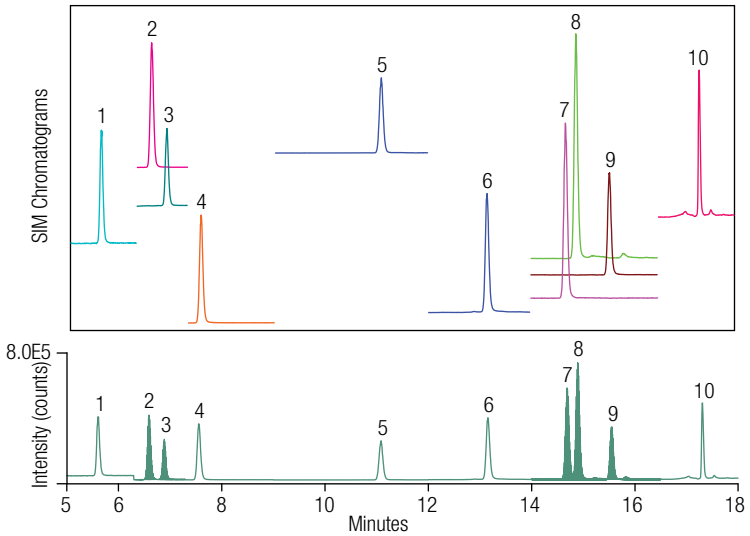

Figure 8-44. Analysis of Carbamate pesticides by LC-MS.

Carbendazim

Carbendazim is a fungicide used in many countries to improve crop production; however, its slow degradation rate and high toxicity may be damaging to human health.

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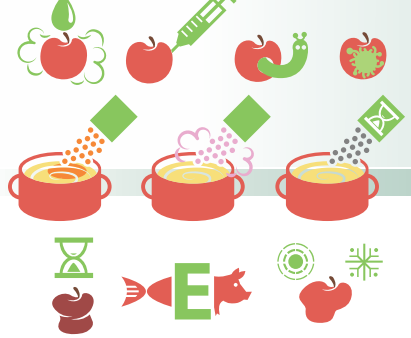

Carbendazim

China regulates the maximum residue limit of carbendazim in foods at 0.5 mg/kg. In the U.S., the Environmental Protection Agency has not approved carbendazim for use as a fungicide on oranges, nor has it established a tolerance,or an exemption from the need for a tolerance, for carbendazim in orange juice. Thus, carbendazim in orange juice is an unlawful pesticide chemical residue under the U.S. Federal Food, Drug, and Cosmetic Act. Therefore, it is necessary to establish efficient analytical methods to detect the presence of the pesticide residue at low concentrations.

Sample preparation is key for the sensitive determination of carbendazim in orange juice, a complex sample matrix. On-line SPE ensures analytical success.

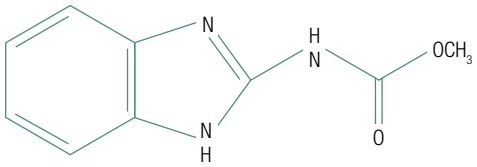

Figure 8-45. Chemical structure of carbendazim.

On-Line SPE

Column:	Acclaim Trinity P1, 3 µm Analytical, 3.0 × 100 mm
Flow:	0.7 mL/min
Injection Volume:	1000 µL onto the on-line SPE cartridge
Mobile Phase:	A, Methanol; B, H_2O
Gradient:	B, 0–2 min, 100%; 2.1–4.5 min, 50%; 6.6–10 min, 100%

Separation

Column:	Acclaim PA2, 3 µm Analytical, 3.0 × 150 mm
Flow:	1.0 mL/min
Temperature :	30 °C
Mobile Phase:	A, Acetonitrile; B, 100 mM Ammonium Acetate
Gradient:	B, 0–3 min, 100%; 6.5 min, 50%; 6.6–10 min, 100%
Detection:	UV absorbance at 285 nm
MSV Time Program:	0 min, 1_2 2.0 min, 6_1 4.5 min, 1_2
Peak:	1. Carbendazim

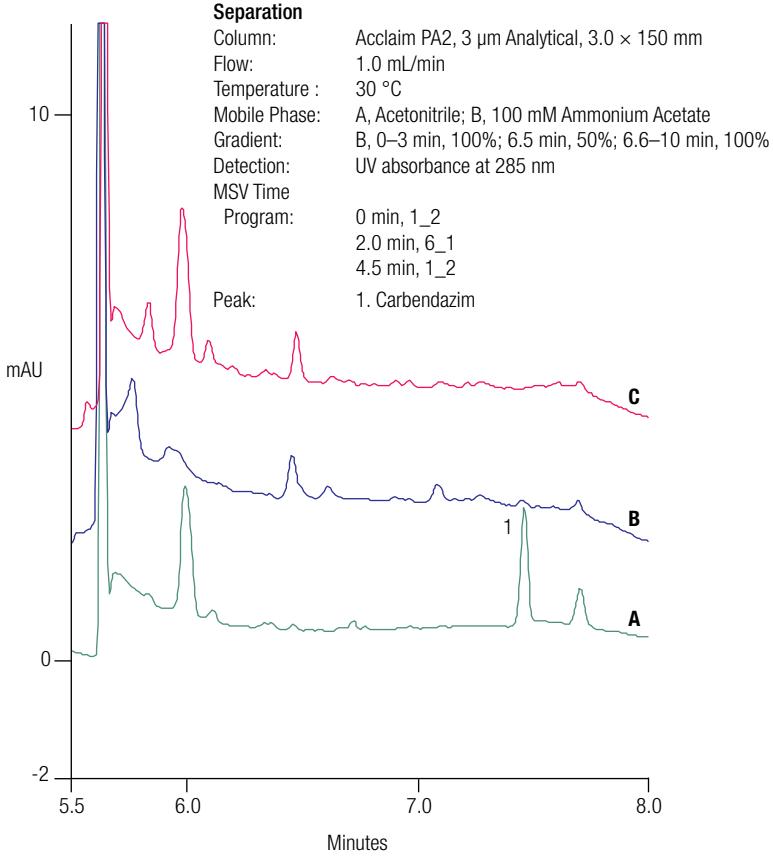

Figure 8-46. Samples of (A) carbendazim standard (5 µg/L), (B) orange juice, and (C) blank.

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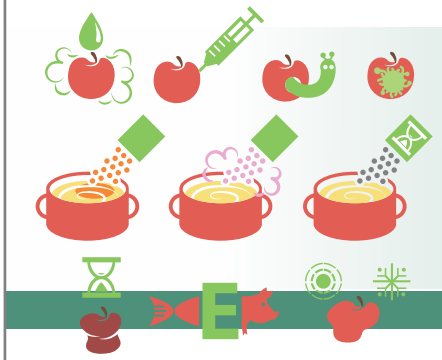

Clenbuterol, Ractopamine, and Phenolethanolamine

Clenbuterol, ractopamine, and phenolethanolamine are β2-agonists that can stimulate the nervous system. They have been extensively used as growth stimulants in farm animals and by athletes seeking enhanced performance.

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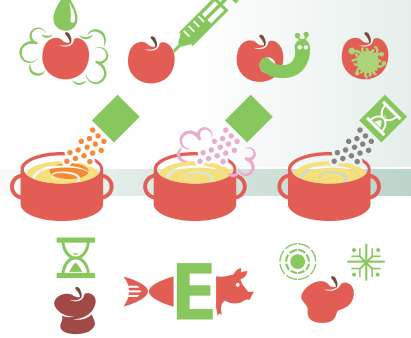

Clenbuterol, Ractopamine, and Phenolethanolamine in Meat

Abuse of clenbuterol, ractopamine, and phenolethanolamine can cause side effects in humans (e.g., increased heart rate and blood pressure, anxiety, palpitation, and skeletal muscle tremors). Therefore, clenbuterol – the most effective β2-agonist used as a growth-promoting agent for farm animals – has been banned as a food/feed additive in many countries, including the USA, European Union (EU), and People's Republic of China. Ractopamine was commercially developed in the USA, where its use is authorized; however, in the EU and People's Republic of China, the use of ractopamine is completely banned.

Phenolethanolamine – recently introduced as a new β2-agonist – already has been banned in the People's Republic of China.

Application Brief 154 discusses a sensitive and rapid HPLC method with on-line SPE and UV detection for simultaneous determination of clenbuterol, ractopamine, and phenolethanolamine in meat.

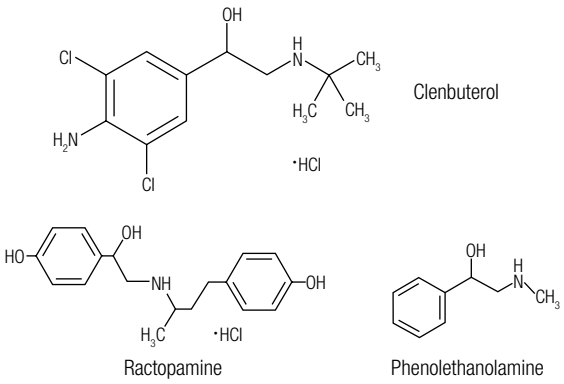

Figure 8-47. Structures of clenbuterol, ractopamine, and phenolethanolamine.

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Download Application Brief 154: Rapid and Sensitive Determination of Clenbuterol, Ractopamine, and Phenolethanolamine in Meat

Clenbuterol, Ractopamine, and Phenolethanolamine in Meat

On-Line SPE Conditions

Cartridge:	Dionex SolEx SPE, 2.1 × 20 mm (P/N 074400), with V-3 Cartridge Holder (P/N 074403)
Mobile Phase:	A: 1.0 mM Na_2HPO_4/4.0 mM NaH_2PO_4/ 0.1 mM $Na_4P_2O_7$ (pH 6, dissolve 0.178 g of $Na_2HPO_4 \cdot 2\ H_2O$, 0.624 g of $NaH_2PO_4 \cdot 2\ H_2O$, and 0.266 g of $Na_4P_2O_7$ in 1 L deionized [DI] water, without pH adjustment) B: CH_3CN
Gradient:	0–3 min, 0% B; 3–6.6 min, 0–50% B; 6.6–8 min, 50% B; 8.1–10 min, 0% B
Flow Rate:	0.4 mL/min
Injection Volume:	2500 µL on the on-line SPE cartridge

Separation Conditions

Column:	Acclaim Polar Advantage, 3 µm Analytical, 3.0 × 150 mm (P/N 063693)
Flow:	0.6 mL/min
Temperature:	25 °C
Mobile Phase:	A. 12.5 mM $HCOONH_4$/50 mM HCOOH (pH 3, dissolve 0.788 g of $HCOONH_4$ and 1.87 mL of HCOOH [99%] in 1 L DI water, without pH adjustment) B. CH_3CN C. H_2O
Gradient:	0–3 min, 20% A, 5% B; 0–3 min, 20% A, 5% B; 3–6.5 min, 20% A, 5–65% B; 6.5–8 min, 20% A, 65% B; 8.1–10 min, 20% A, 5% B
Detection:	UV, absorbance at 210 nm
Valve Position:	0 min, 1_2; 2.9 min, 6_1; 8 min, 1_2
Samples:	A. Mixture of standards (200 µg/L each) B. Pork
Peaks:	1. Clenbuterol 2. Ractopamine 3. Phenolethanolamine

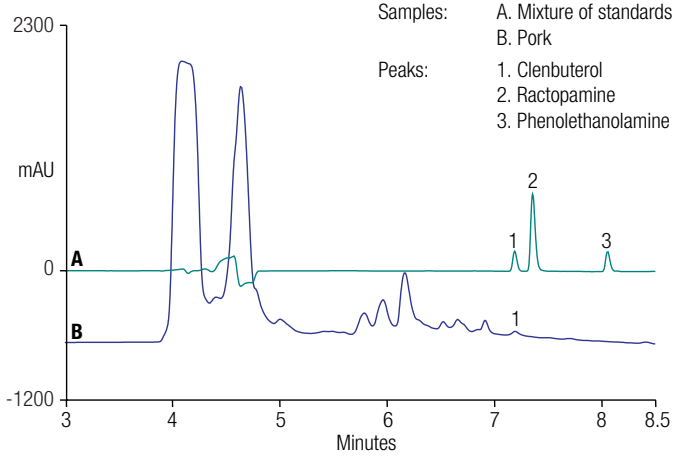

Figure 8-48. (A) A mixture of standards and (B) an extracted pork sample.

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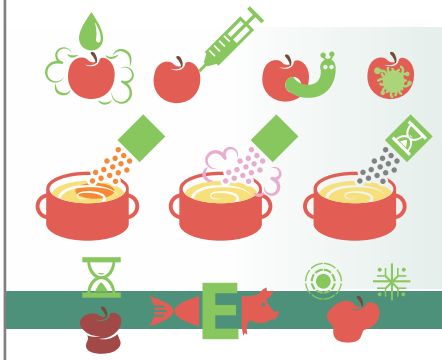

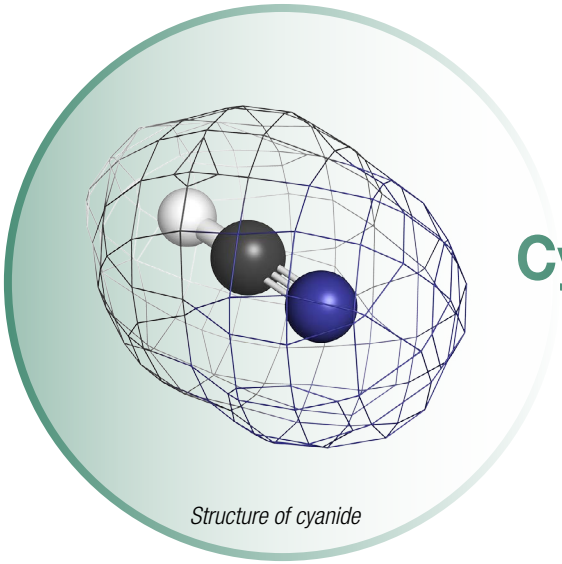

Structure of cyanide

Cyanide

Cyanide is a well known acute toxin that prevents cellular respiration by irreversibly binding with the iron in cytochrome C oxidase. In addition, thiocyanate, which is metabolized from cyanide, interferes with iodine uptake by the thyroid gland, causing goiters and other long-term iodine deficiency diseases.

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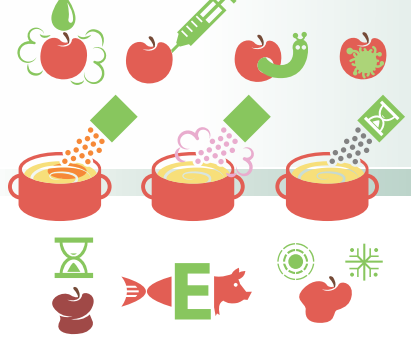

Cyanide

Cyanide occurs naturally in many foods (cassava, sorghum, African lima beans, bamboo shoots, bitter almonds, and apricot, cherry, and peach pits) and is naturally generated by microorganisms. Cyanide is used in many industries (e.g., plating and mining) and it can be released into the air from burning coal and plastics. In the U.S., drinking water contamination with cyanide is typically from an industrial source or leached from waste sites.

Cyanide is regulated as an environmental contaminant by the United States Environmental Protection Agency (EPA) for drinking water, surface water, and wastewater due to these health concerns. Total cyanide is defined by the EPA as free cyanide ion and complex cyanides that are converted to hydrocyanic acid (HCN) during strong acid digestion. More recently, total cyanide also includes ferrocyanide and ferricyanide due to free cyanide formed by exposure to light. For drinking and surface waters, the EPA has established a maximum contamination level (MCL) of 200 µg/L free cyanide determined by a total cyanide assay. To determine total cyanide, the sample is digested with sulfuric acid to convert the cyanide to hydrogen cyanide gas, aspirated into a strong caustic solution, then assayed.

Application Notes 173 and 227 describe ion chromatography with pulsed amperometric detection methods for the determination of cyanide in drinking water.

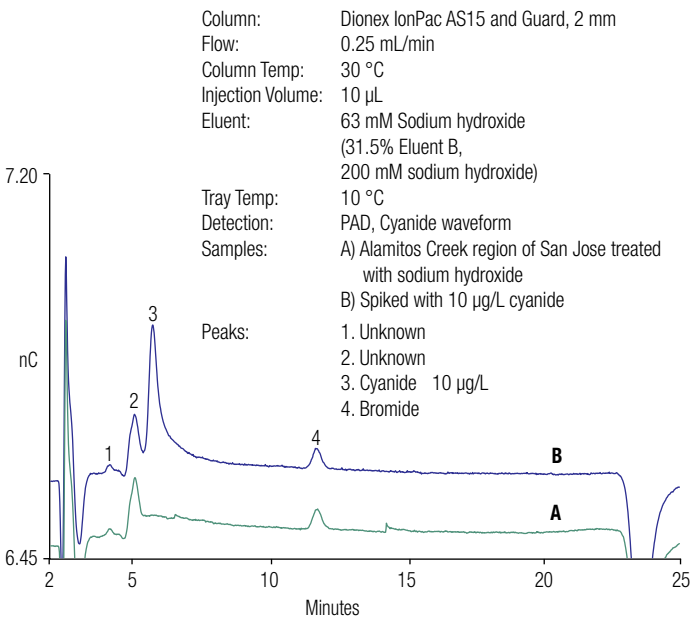

Figure 8-49. Treated city of San Jose drinking water with and without 10 µg/L of cyanide.

Download Application Note 173: Direct Determination of Cyanide in Drinking Water by Ion Chromatography with Pulsed Amperometric Detection

Download Application Note 227: Determination of Total Cyanide in Municipal Wastewater and Drinking Water Using Ion-Exclusion Chromatography with Pulsed Amperometric Detection (ICE-PAD)

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Cyanide

Column: Dionex IonPac AS15 and Guard, 2 mm
Flow: 0.25 mL/min
Column Temp: 30 °C
Injection Volume: 10 µL
Eluent: 63 mM Sodium hydroxide (31.5% Eluent B, 200 mM sodium hydroxide)
Tray Temp: 10 °C
Detection: PAD, Cyanide waveform
Samples: A) City of Sunnyvale drinking water (sampled in the fall), treated
B) Sample A spiked with 10 µg/L cyanide

Peaks: 1. Unknown
2. Chloride
3. Cyanide 10 µg/L
4. Unknown

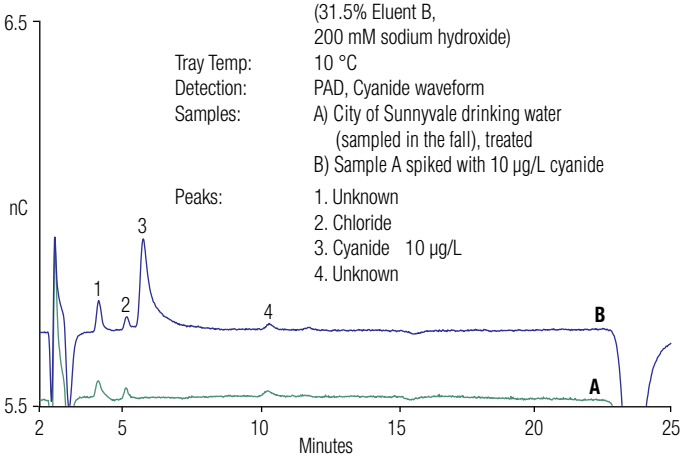

Figure 8-50. Treated city of Sunnyvale drinking water with and without 10 µg/L of cyanide.

Did You Know?

Cyanide is released from natural food substances, including lima beans and almonds. It is also found in the pits of various fruits including peaches, apricots, and apples.

Column: Dionex IonPac ICE-AG1, Dionex IonPac ICE-AS1 (4 mm)
Flow: 0.2 mL/min
Temperature: 30 °C
Injection Volume: 50 µL
Eluent: 50 mM methanesulfonic acid
Detection: PAD, Pt (Disposable)
Sample Prep.: MICRO DIST acid digestion
Samples: A: Municipal drinking water + base
B: Sample A + 1 µg/L cyanide

Peaks:	A	B	
1. Unknown	—	—	µg/L
2. Cyanide	0.67	1.61	
3–5. Unknown	—	—	

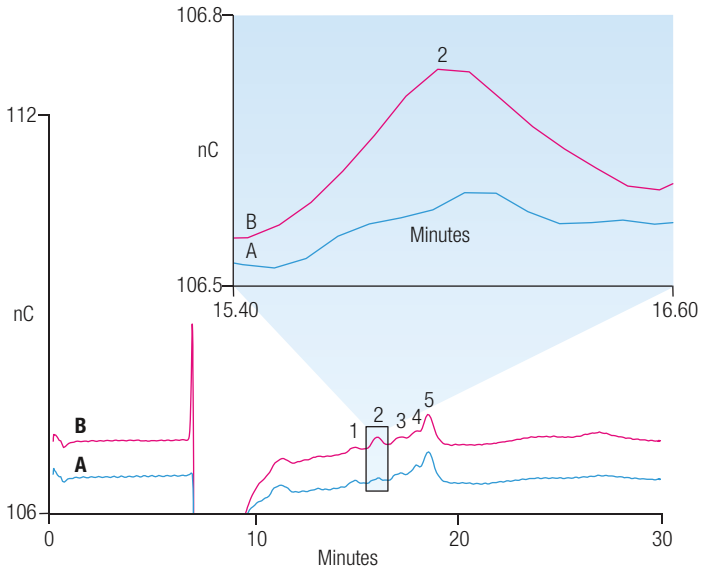

Figure 8-51. Comparison of A) Municipal drinking water and B) Sample A with 1 µg/L cyanide added.

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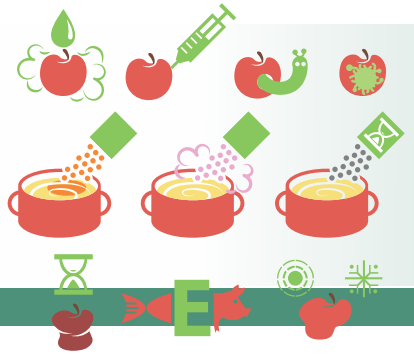

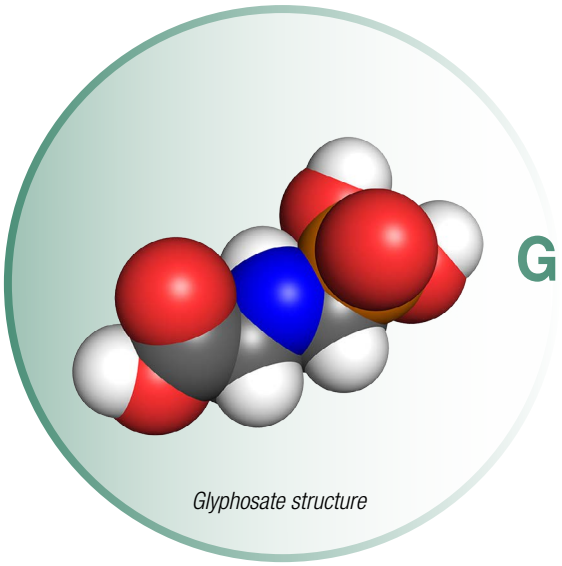

Glyphosate structure

Glyphosate

Glyphosate is a broad-spectrum herbicide with low mammalian toxicity. The herbicide's widespread use makes it a possible contaminant in ground water and eventually drinking water.

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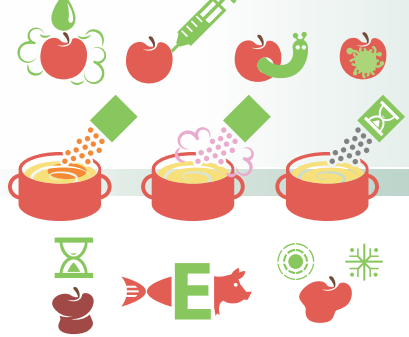


Glyphosate

The U.S. EPA has established Method 547 to monitor glyphosate in drinking water. Glyphosates can also contaminate plants used in botanical supplements.

This application details a convenient chromatographic method for the analysis of glyphosate and its primary metabolite, aminomethylphosphonic acid (AMPA). Because glyphosate has been shown to rapidly decompose in chlorinated water, AMPA is the species most likely to be found in drinking water matrices.

Column :	Glyphosate Column, cation exchange, 4 mm × 150 mm, 8 µm and guard, cation exchange, 3 mm × 20 mm × 8 µm
Flow:	0.40 mL/min
Temperature:	55 °C
Eluents:	A: Potassium phosphate; B: Potassium hydroxide
Gradient:	Time (min): A (%) B (%) 0 100 0 15 100 0 15.01 0 100 17 100 0 25 100 0
Postcolumn Reagent 1:	Oxidizing reagent at 36 °C
Flow Rate:	0.300 mL/min
Reagent 2:	OPA reagent, ambient
Flow Rate:	0.300 mL/min
Fluorescence:	Excitation: 330 nm Emission: > 460 nm (cut-off filter)
Peak:	1. Glyphosate 0.84 mg/mL

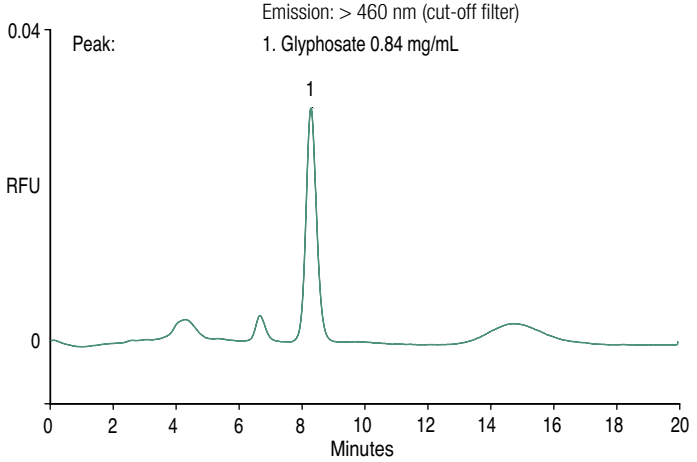
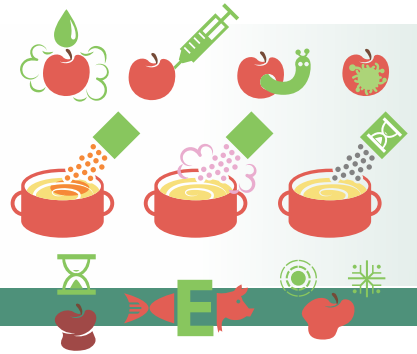


Figure 8-52. Glyphosate in a milkweed sample. Total concentration of glyphosate = 23 µg/g of plant material. Injection volume = 50 µL.



Gutter Oil

Cooking oils come from a variety of sources, including olive, rapeseed, peanut, grapeseed, mustard, corn, and many others. Gutter oil is a term used to describe illicit cooking oil which has been recycled from waste oil collected from sources such as restaurant fryers, sewer drains, and slaughter houses. Cooking oil must be monitored for quality and contamination.

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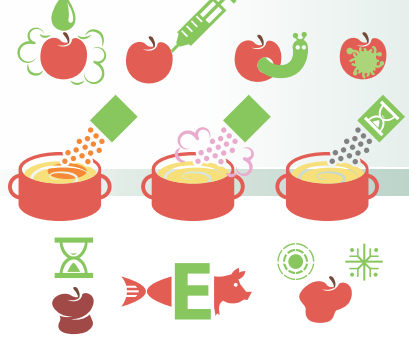


Gutter Oil

When cooking oil is heated, it can undergo many chemical changes including oxidation of unsaturated fatty acids, triglyceride decomposition, and the formation of potentially cytotoxic oxidation products such as 4-hydroxy-trans-2-nonenal (HNE) and other aldehydes. Rancidity during long term storage can also occur and is associated with the content of polyunsaturated fatty acid content. Although these issues make used oil unfit for use in the kitchen, and unhealthy for human consumption, it can still act as a useful resource as a raw material for biofuels production. As there is a significant price difference between high quality cooking oils and lower quality biofuel raw materials, the possibility exists for unscrupulous people to filter and decolorize used cooking oils and sell them as high quality cooking oils. Such treated used oils are referred to as gutter oils (GO). Poster Note 70536 describes HPLC Charged Aerosol Detection based methods to identify GOs from cooking oils, based on the lipid profiles.

Download Poster Note: Characterization of Used Cooking Oils by High Performance Liquid Chromatography and Corona Charged Aerosol Detection

Gutter Oil

HPLC Column:	Accucore C8, 2.6 µm 4.6 × 150 mm HPLC
Flow:	Elution pump: 0.8 mL/min, Inverse gradient pump: 1.2 mL/min
Column Temp.:	40 °C
Injection Volume:	5 µL
Mobile Phase:	A: Methanol/water/acetic acid (650:350:4) B: Acetonitrile C: Isopropyl alcohol
Nebulizer Temperature:	20 °C
Sample Temperature:	20 °C
Gradient:	See below

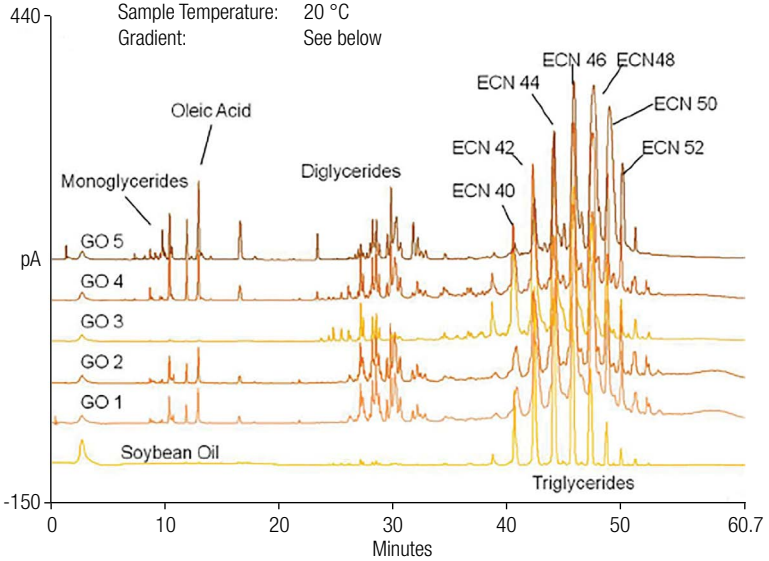


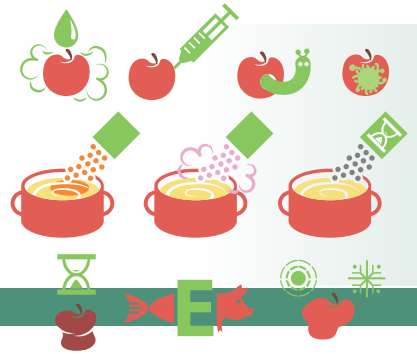
Figure 8-53. HPLC-Corona charged aerosol detector chromatogram of unused soybean oil and five gutter oils, normalized to the equivalent carbon number (ECN) 46 peak. While soybean oil is primarily composed of triglycerides, GOs also contain free fatty acids, monoglycerides, and diglycerides.

Table 8-6. Elution gradient.

Time (min)	%A	%B	%C
-5.0	100	0	0
0.0	100	0	0
1.0	100	0	0
2.0	50	50	0
15.0	45	55	0
23.0	0	100	0
30.0	0	100	0
60.0	0	35	65

Table 8-7. Inverse gradient.

Time (min)	%A	%B	%C
-5.0	0.0	66.7	33.3
0.0	0.0	66.7	33.3
1.7	0.0	66.7	33.3
2.7	33.3	33.3	33.3
15.7	40.0	26.7	33.3
23.7	66.7	0.0	33.3
30.7	66.7	0.0	33.3
60.7	66.7	33.3	0.0



Hexavalent Chromium

Hexavalent chromium, Cr(VI), is the most toxic form of the metal chromium, a primary drinking water contaminant in the U.S.

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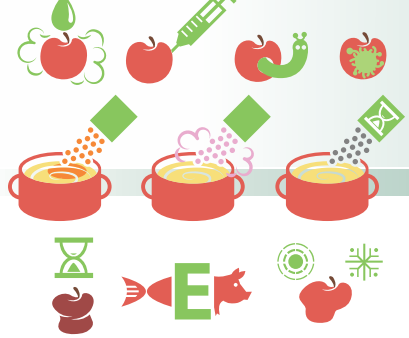

Hexavalent Chromium

Dissolved hexavalent chromium can be determined as chromate (CrO_4^{2-}) by ion chromatography in drinking water, groundwater, and industrial wastewater effluents as described in U.S. EPA Method 218.6 and Dionex, now part of Thermo Scientific, Technical Note 26. Technical Note 26 uses a 250-µL injection onto a high-capacity Dionex IonPac AS7 anion exchange column to separate Cr(III) from Cr(VI) in four minutes. The product of the postcolumn reaction between Cr(VI) and diphenylcarbazide is detected by absorbance at 530 nm, yielding a method detection limit of 0.4 µg/L in reagent water.

The California Department of Health Services (DHS) issued a Public Health Goal (PHG) of 2.5 µg/L for total chromium and 0.2 µg/L for Cr(VI). In January 2001, California DHS added Cr(VI) to the list of unregulated chemicals that must be monitored. As a result of this regulation, public water systems are monitoring Cr(VI) in drinking water. EPA Method 218.6 does not allow sufficient sensitivity for analysis at the California PHG level of 0.2 µg/L. Thermo Scientific Application Update 144 describes modifications to Method 218.6 that significantly increase sensitivity over the existing method. The modifications include lower eluent and postcolumn reagent (PCR) flow rates, a larger reaction coil, and a larger injection volume. The resulting MDL for Cr(VI) as CrO_4^{2-} of 0.02 µg/L is more than sufficient for determinations at the California PHG level.

More recently, Thermo Fisher Scientific designed an even more sensitive Cr(VI) assay that resulted in the US EPA Method 218.7. This work is detailed in Application Update 179.

Column:	Dionex IonPac, NG1, AS7		
Flow:	1.0 mL/min		
Injection Volume:	1000 µL		
Eluent:	250 mM $(NH_4)_2SO_4$, 100 mM NH_4OH		
Post-column Reagent:	2 mM diphenylcarbazide, 10% CH_3OH, 1N H_2SO_4		
RXN Coil:	750 µL		
Detector:	UV/Vis (530 nm)		
Sample:	Sunnyvale, CA tap water spiked with 0.2 µg/L Cr(VI)		
		A	B
Peaks:	1. Chromate	0.055 µg/L	0.245 µg/L

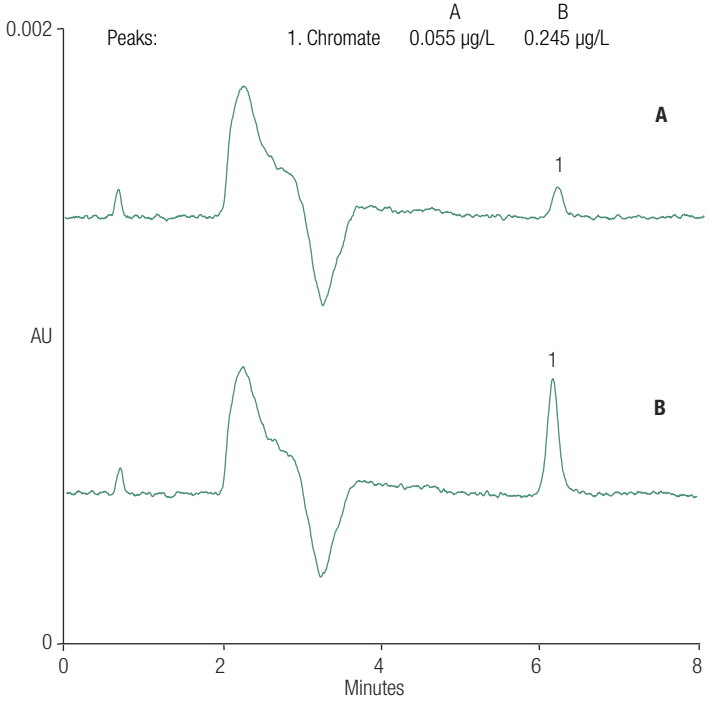

Figure 8-54. Determination of chromate in drinking water.

Download Technical Note 26: Determination of Cr(VI) in Water, Waste Water, and Solid Waste Extracts

Download Application Update 144: Determination of Hexavalent Chromium in Drinking Water Using Ion Chromatography

Download Application Update 179: Sensitive Determination of Hexavalent Chromium in Drinking Water

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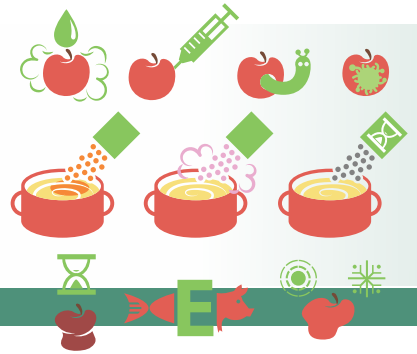

Hydroxymethylfurfural

Hydroxymethylfurfural (HMF), or 5-hydroxymethyl-2-furaldehyde, is a water-soluble heterocyclic organic compound derived from sugars. Very low amounts of this compound are naturally found in fresh sugar-containing foods including milk, honey, fruit juices, spirits, and bread.

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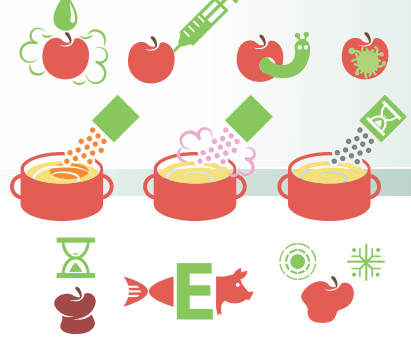


Hydroxymethylfurfural

Besides occurring naturally, HMF is produced during food pasteurization and cooking as a result of dehydration of sugars such as glucose and fructose and in the initial stages of the Maillard reaction, a reaction between sugars and proteins responsible for changes in color and flavor of food. HMF is also formed during extended food storage under acidic conditions that favor its generation. Therefore, it is an indicator of excessive heat-treatment, spoilage, and of possible adulteration with other sugars or syrups.

Although HMF is not yet considered a harmful substance, the National Institute of Environmental Health Sciences nominated HMF for toxicity testing based on the potential for widespread exposure through consumed foods, and evidence for carcinogenic potential of other members of this class. As a result, many countries impose restrictions on maximum levels of HMF in food and beverages.

Application Note 270 describes a high-performance anion-exchange chromatography with pulsed amperometric detection (HPAE-PAD)-based method for the determination of HMF in samples ranging from food (honey and pancake syrup) to treated biomass (corn stover and wood acid hydrolysate).

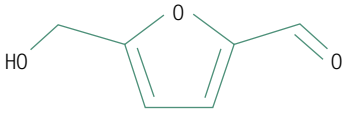


Figure 8-55. 5-Hydroxymethylfurfural structure.

Column:	Thermo Scientific™ Dionex™ CarboPac™ PA1, Analytical, 4 × 250 mm Dionex CarboPac PA1, Guard, 4 × 50 mm	Peaks:		
		1. Glycerol	–	µg/mL
		2. HMF	3.4	
		3. Glucose	–	
Flow:	1.0 mL/min	4. Xylose	–	
Temperature:	30 °C	5. Fructose	–	
Injection Volume:	10 µL (full loop)	6. Sucrose	–	
Eluent:	50 mM KOH			
Eluent Source:	Dionex EGC II KOH Cartridge			
Detection:	PAD (Au)			

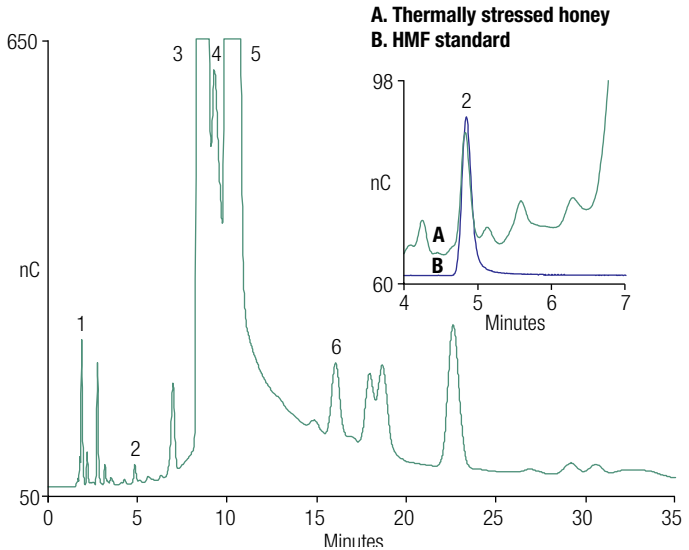
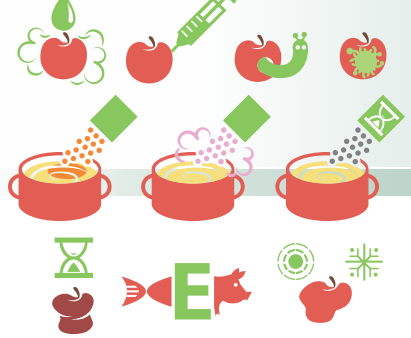


Figure 8-56. HMF in thermally stressed honey.



Hydroxymethylfurfural

Column:	Dionex CarboPac PA1, Analytical, 4 × 250 mm Dionex CarboPac PA1, Guard, 4 × 50 mm	
Flow:	1.0 mL/min	
Temperature:	30 °C	
Injection Volume:	10 µL (full loop)	
Eluent:	50 mM KOH	
Eluent Source:	Dionex EGC II KOH cartridge	
Detection:	PAD (Au)	
Peaks:	1. Glycerol	– µg/mL
	2. HMF	0.42
	3. Glucose, Fructose	–
	4. Sucrose	–

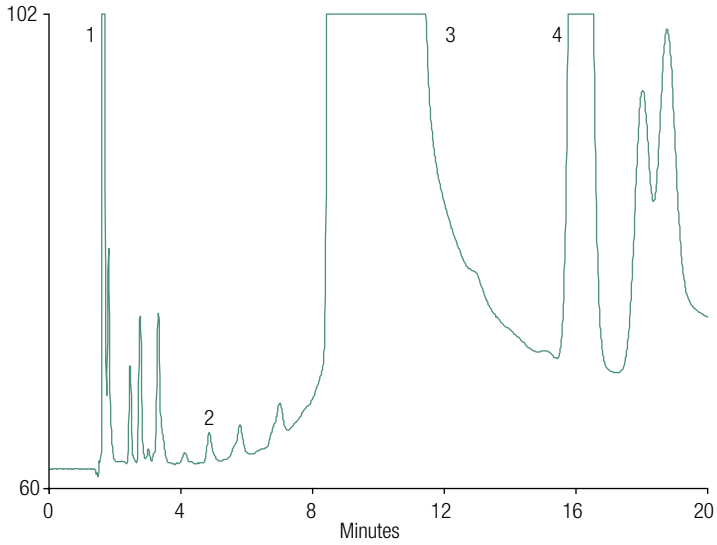


Figure 8-57. HMF in pancake syrup (high-fructose corn syrup).

Did You Know?

- HMF can be used as an indicator of excessive heat treatment
- HMF is also found in cigarette smoke and glucose syrup.

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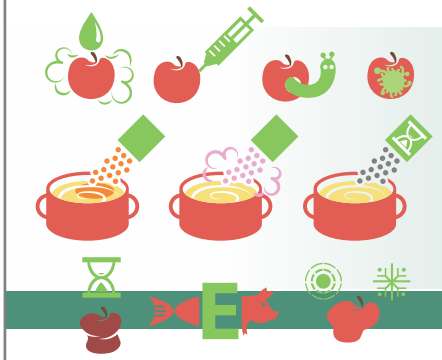

Inorganic Anions in Drinking Water

The determination of common inorganic anions in drinking water is one of the most important applications of ion chromatography worldwide. The National Primary Drinking Water Standards in the United States specify a Maximum Contaminant Level (MCL) for a number of inorganic anions, including fluoride, nitrite, and nitrate.

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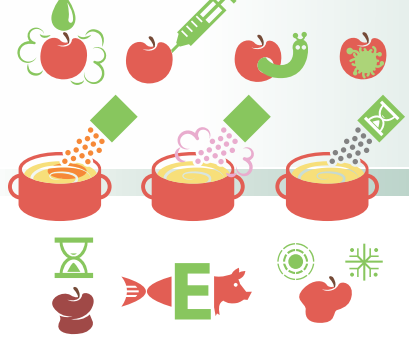


Inorganic Anions in Drinking Water

Maximum Contaminant Levels (MCLs) are specified to minimize potential health effects arising from the ingestion of these anions in drinking water. High levels of fluoride cause skeletal and dental fluorosis, and nitrite and nitrate can cause methemoglobulinemia, which can be fatal to infants. Other common anions, such as chloride and sulfate, are considered secondary contaminants. The National Secondary Drinking Water Standards in the U.S. are guidelines regarding taste, odor, color, and certain aesthetic characteristics. Although these guidelines are not federally enforced, they are recommended to all states as reasonable goals and many states adopt their own regulations governing these contaminants.

Ion chromatography (IC) has been approved for compliance monitoring of these common inorganic anions in U.S. drinking water since the mid-1980s, as described in U.S. EPA Method 300.0. Application Notes 133 and 140 describe IC with suppressed conductivity methods for ion analysis in drinking water that are consistent with U.S. EPA Method 300.0.

U.S. EPA Method 300.0 (Part A) describes the use of a Dionex IonPac AS4A anion-exchange column using a carbonate/bicarbonate eluent and suppressed conductivity detection for the determination of inorganic anions in environmental waters, such as drinking water, wastewater (mixed domestic and industrial), groundwater, and aqueous solid extracts. However, the method allows for alternative columns, eluents, suppression devices, and detectors to be used—provided that equivalent or better performance for the method is obtained and that the quality assurance requirements are met, including an initial demonstration of capability.

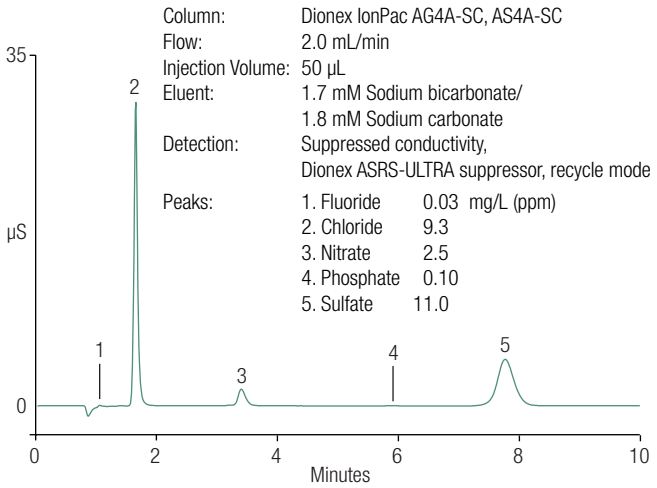


Figure 8-58. Determination of inorganic anions in drinking water using a Dionex IonPac AS4A-SC column.

Download Application Note 133: Determination of Inorganic Anions in Drinking Water by Ion Chromatography

Download Application Note 140: Fast Analysis of Anions in Drinking Water by Ion Chromatography

Inorganic Anions in Drinking Water

Column:	Dionex IonPac AG14A, AS14A, (3 mm)
Flow:	0.8 mL/min
Temperature:	30 °C
Injection Volume:	25 µL
Eluent:	8.0 mM Sodium carbonate/1.0 mM Sodium bicarbonate
Detection:	Suppressed conductivity, Dionex AAES suppressor, recycle mode, 45 mA
Peaks:	1. Fluoride 0.05 mg/L (ppm) 2. Chloride 42 3. Bromide 0.03 4. Nitrate 2.6 5. Phosphate 0.5 6. Sulfate 37

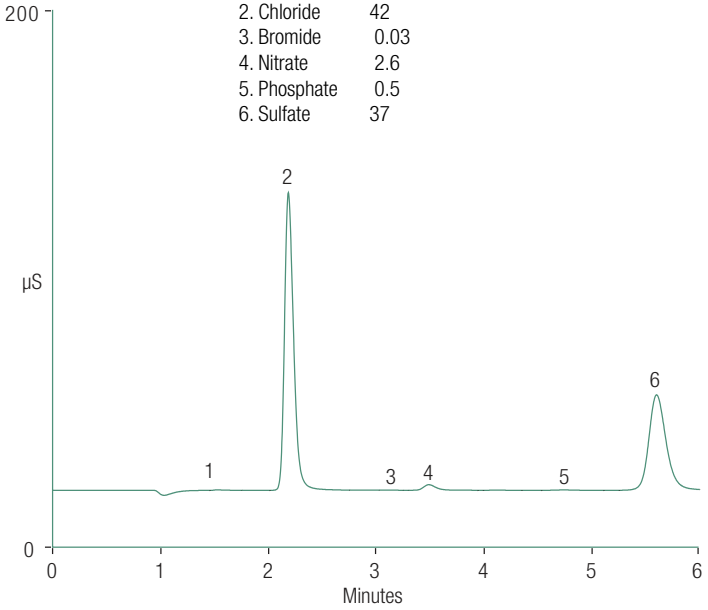
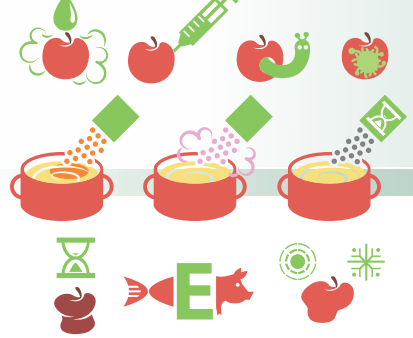


Figure 8-59. Anions in Sunnyvale, CA drinking water separated using the Dionex IonPac AS14A column (3 mm) at 0.8 mL/min.

Table 8-8. Summary of drinking water samples using the AS14A (3 mm) column at 0.8 mL/min flow with the Thermo Scientific™ Dionex™ Atlas™ Suppressor.

	Sunnyvale 8/8/00 (ppm)	Sunnyvale 2/22/0 (ppm)	Palo Alto 2/21/01 (ppm)	Twain Harte 2/20/01 (ppm)
Fluoride	0.047	0.052	0.728	0.016
Chloride	16.6	42.1	4.1	3.5
Nitrite	< 0.003	< 0.003	< 0.003	< 0.003
Bromide	0.021	0.033	<0.004	<0.004
Nitrate	1.91	2.60	0.17	0.066
Phosphate	0.328	0.483	<0.010	<0.010
Sulfate	18.8	36.8	6.45	0.228



Inorganic Anions in Drinking Water

Traditionally, columns designed for use with carbonate/bicarbonate eluents have been used for determining inorganic anions in environmental samples. Columns that use hydroxide eluents (i.e., hydroxide selective columns) have not been as widely used for routine analysis of inorganic anions in environmental waters due to the lack of appropriate selectivity and difficulty in preparing contaminant-free hydroxide eluents. The introduction of automated, electrolytic eluent generation has eliminated the difficulty in preparing hydroxide eluents. A hydroxide-selective column, the Dionex IonPac AS18, was developed to determine inorganic anions in environmental waters. In Application Note 154 the use of automated eluent generation, combined with a high-capacity, hydroxide-selective, anion-exchange column – the Dionex IonPac AS18 – for the determination of inorganic anions in environmental waters is described.

Column:	Dionex IonPac AG18, AS18, 4 mm	
Flow:	1.0 mL/min	
Temperature:	30 °C	
Injection Volume:	25 µL	
Eluent:	22–40 mM KOH from 7–8 min	
Eluent Source:	ICS-2000 with CR-ATC	
Detection:	Dionex ASRS ULTRA suppressor, 4 mm, recycle mode	
Peaks:	1. Fluoride	0.07 mg/L (ppm)
	2. Chloride	45.3
	3. Nitrite-N	0.02
	4. Carbonate	–
	5. Bromide	0.03
	6. Sulfate	58.7
	7. Nitrate-N	0.65
	8. Phosphate-P	0.47

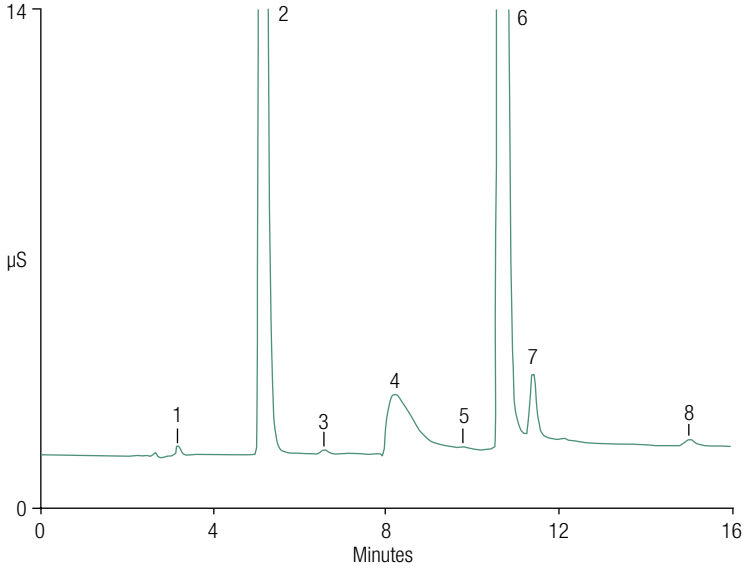


Figure 8-60. Determination of inorganic anions in Sunnyvale, CA, drinking water using the Dionex IonPac AS18 column.

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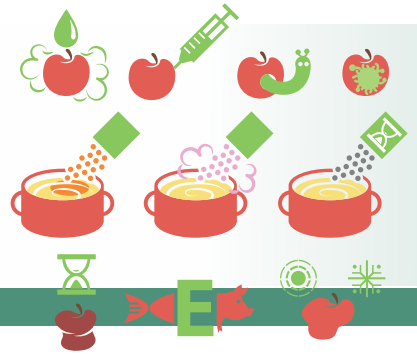
Download Application Note 154: Determination of Inorganic Anions in Environmental Waters Using a Hydroxide-Selective Column



Microcystins

Waterblooms of cyanobacteria (blue-green algae) can produce potent toxins that have become a severe problem for eutrophic aquatic environments. Hepatotoxins are among the primary toxins produced by these species growing in lakes, ponds, and rivers used as drinking water sources. Microcystins are cyclic non-ribosomal peptide hepatotoxins that exhibit tumor-promoting activity and are among the most commonly found cyanobacteria toxins.

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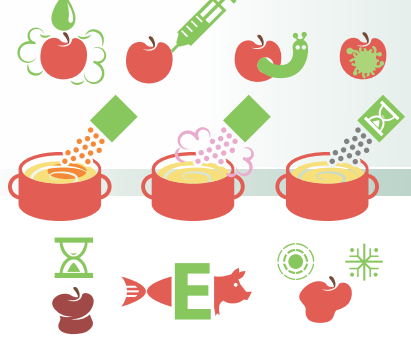


Microcystins

Microcystin contamination of drinking water at low nanomolar concentrations is considered a risk factor for cancer, and microcystin-LR has been associated with most of the incidents of toxicity involving microcystins. Therefore, the World Health Organization (WHO) has proposed a provisional guideline concentration of 1.0 µg/L for microcystin-LR in drinking water.

This application uses a target-cut on-line SPE method followed by HPLC with UV detection for the determination of three microcystins (-LR, -RR, and -YR) in drinking, tap, and lake water. The three target analytes were co-eluted from the first column using chromatographic conditions that eliminated as many interferences as possible; then the analytes were sent to the analytical flow path and separated on the second column using the same type of stationary phase under different chromatographic conditions. This design takes advantage of the separation power of both columns and may eliminate interferences more efficiently than typical on- and off-line SPE methods.

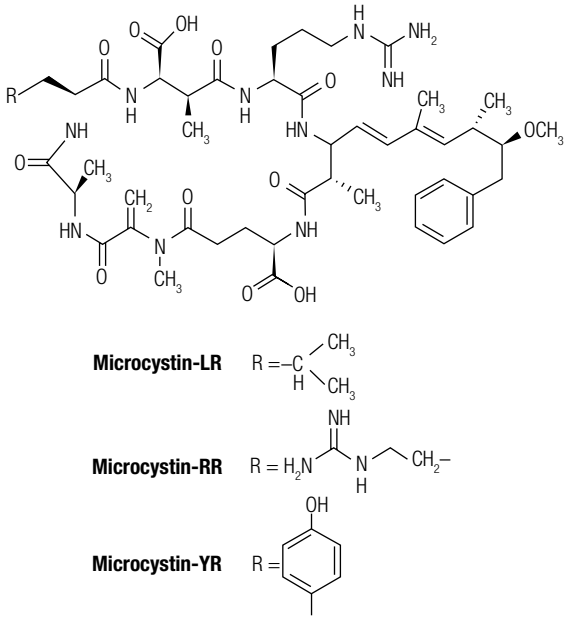
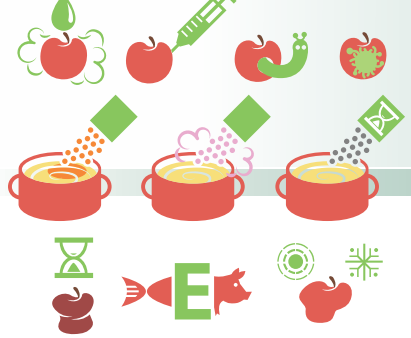


Figure 8-61. Chemical structures of various microcystins.



Microcystins

SPE Column:	Acclaim PA2, 3 µm, 3.0 × 33 mm
Anal. Column:	Acclaim PA2, 3 µm, 3.0 × 150 mm
Flow:	0.7 mL/min for SPE and separation
Column Temp.:	40 °C
Injection Volume:	2500 µL on SPE column
Eluent for SPE:	CH_3CN–phosphate buffer (22.5 mM KH_2PO_4–2.5 mM K_2HPO_4) In gradient: CH_3CN, 0–5 min, 20%; 7.0 min, 35%; 12min, 59%; 12.1–15 min, 15%
Eluent for Separation:	CH_3CN–0.05% (v/v) H_3PO_4 In gradient: CH_3CN, 0–7.0 min, 15%; 7.5–8.5 min, 80%; 8.6–15 min, 20%
Detection:	UV at 240 nm
Samples:	A. Tap water B. Lake water C. Bottled spring water

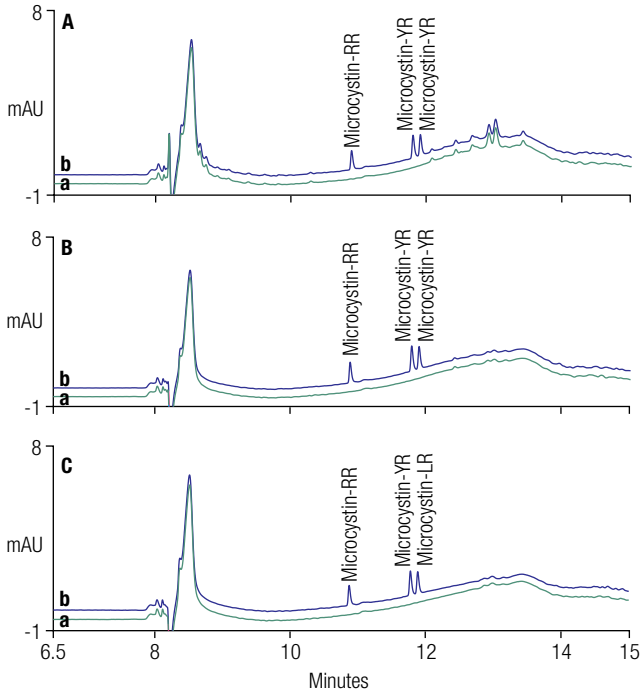
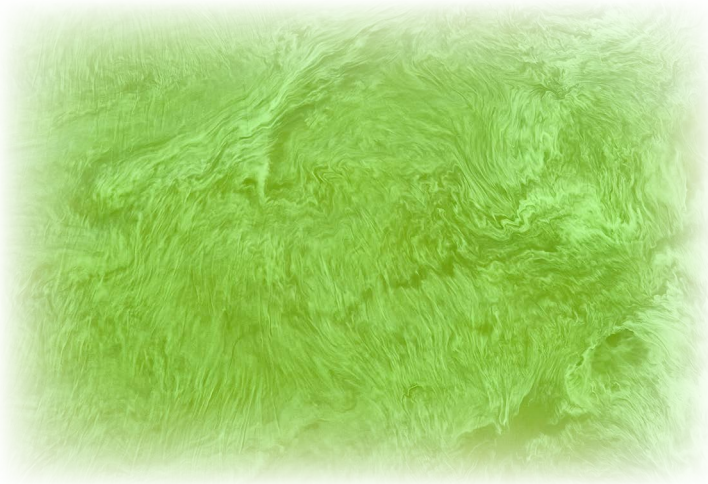


Figure 8-62. Overlay of chromatograms for a) water sample and b) the same sample spiked with 0.5 µg/L each of microcystin-RR, -YR, and -LR standard



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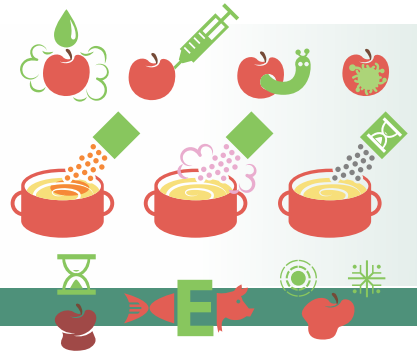

Nitrate and Nitrite

Whether added to processed meat products to protect against microorganisms that can cause food poisoning, or as a contaminant in the water used to make infant formula, exposure to nitrate and nitrite can be associated with health problems. Accordingly, levels of these anions need to be monitored and their content in foods and beverages kept below defined limits.

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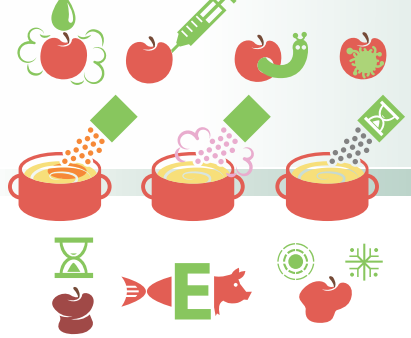


Nitrate and Nitrite in Meats

Nitrate and nitrite are usually added to processed meat products to protect against microorganisms that can cause food poisoning, such as Clostridium botulinum. However, nitrite can react with secondary amines to form nitrosoamines, a class of carcinogenic compounds, in food products or in the digestive system. Nitrate, although more stable than nitrite, can act as a reservoir for nitrite, as nitrate can readily be converted into nitrite by microbial reduction. Thus, both nitrate and nitrite must be monitored to ensure the quality and safety of meat products. This application describes an accurate and sensitive method in which nitrate and nitrite are extracted from meat products and then determined directly using anion exchange chromatography with UV detection. Commercially available ham and salami were used as model samples.

Column:	Dionex IonPac AS11 (4 x 250 mm) and AG11 guard (4 x 50 mm)
Flow Rate:	1 mL/min
Injection Volume:	25 µL
Eluent:	A: 50 mM Sodium hydroxide B: Deionized water C: 100 mM Sodium hydroxide
Detection:	UV, 225 nm
Peaks:	1. Nitrite 1.16 mg/L 2. Nitrate 0.54

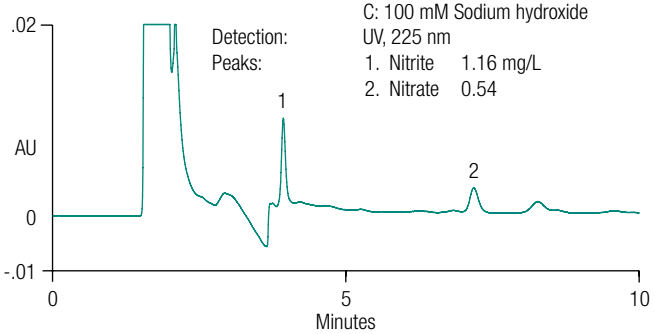


Figure 8-63. Separation of nitrate and nitrite from ham.

Column:	Dionex IonPac AS11 (4 x 250 mm) and AG11 guard (4 x 50 mm)
Flow Rate:	1 mL/min
Injection Volume:	25 µL
Eluent:	A: 50 mM Sodium hydroxide B: Deionized water C: 100 mM Sodium hydroxide
Detection:	UV, 225 nm
Peaks:	1. Nitrite 9.85 mg/L 2. Nitrate 10.8

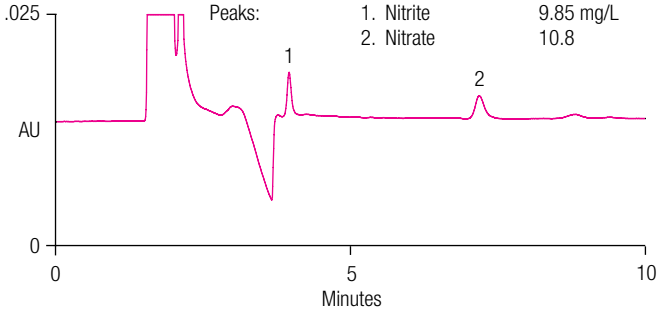
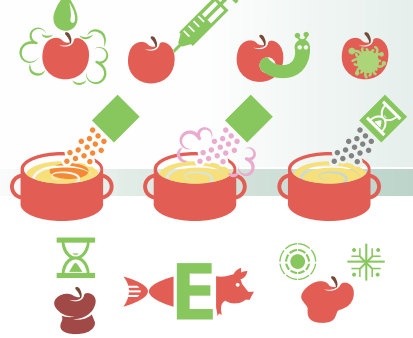


Figure 8-64 Separation of nitrate and nitrite from salami. The extract was diluted fourfold before injection.



Nitrate and Nitrite in Milk

Cow's milk is of particular dietary value to infants, small children, and expectant mothers as it is an important source of calories, minerals (including calcium), fat-soluble vitamins and protein. Because of its nutritional value, it is imperative that the commercial milk supply be free of contaminants such as nitrate and nitrite. The excessive consumption of nitrate can lead to underoxygenation of the blood and tissues, which can cause numerous health problems and even death. With a much smaller total blood volume, infants and small children are more severely impacted than adults when consuming the same nitrate-contaminated product. The most likely source of nitrate in the blood stream is drinking water. Drinking water can become contaminated in areas where there has been excessive application of nitrate-based fertilizers and where sodium or potassium nitrate is used to kill rodents. For an infant, the water used to prepare infant formula (baby food), the water consumed by the nursing mother, or the water consumed by dairy cattle whose milk is used to prepare milk-based infant formulas, are possible sources of nitrate. For most children, infant formula and mother's milk will eventually be replaced by cow's milk.

Nitrite is also a concern because it is easily oxidized to nitrate. Excessive consumption of nitrite and nitrate also has been implicated as a cause of other health problems. For these reasons, the United States Environmental Protection Agency (U.S. EPA) regulates the amount of nitrite and nitrate in drinking water and has published an ion chromatography method.

Column:	Dionex IonPac AS20 Analytical, 4 × 250 mm Dionex IonPac AG20 Guard, 4 × 50 mm
Flow:	1.0 mL/min
Column Temp.:	30 °C
Injection Volume:	25 µL
InGuard:	HRP, 9 × 24 mm
Concentrator:	Dionex IonPac UTAC-LP1, 4 × 35 mm
Eluent Source:	EGC II KOH with CR-ATC
Gradient:	Time (min) Eluent Conc. (mM) -20 50 -7.1 50 -7.0 7 -5.0 7 0.0 7 25.0 7 25.1 50
Detection:	Suppressed conductivity, Dionex ASRS 300 suppressor, 4 mm with external water mode, current 125 mA
Sample:	A. Sample #1 B. Spiked Sample #1

Peaks:	Conc. (mg/L) A	B
1. Nitrite	ND	0.017
2. Nitrate	0.020	0.065

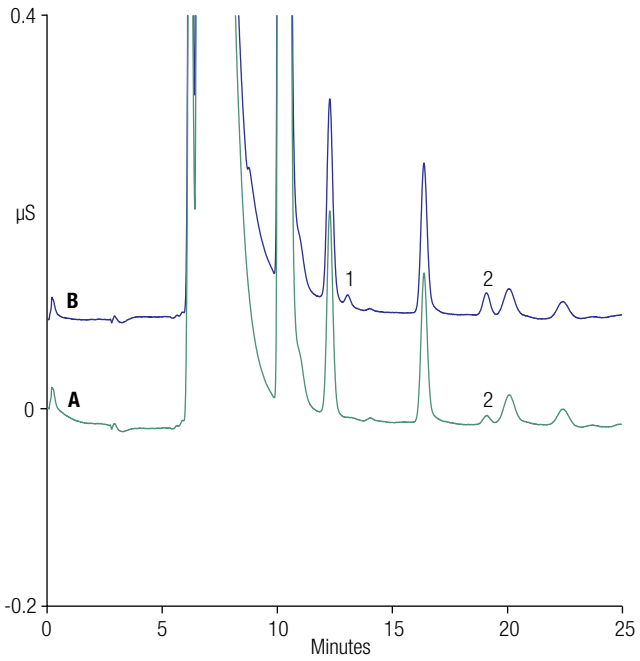


Figure 8-65. Overlay of chromatograms of Milk Sample #1 and Spiked Milk Sample #1.

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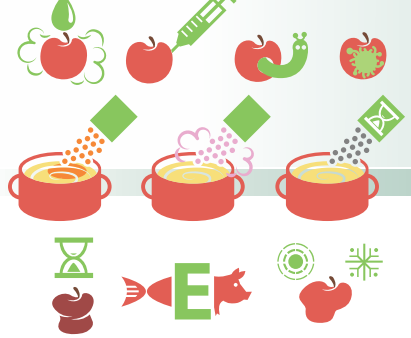


Nitrate and Nitrite in Milk

Application Note 279 describes the routine measurement of nitrate and nitrite in acid precipitated milk samples using ion chromatography with UV and suppressed conductivity detection.

Column:	Dionex IonPac AS20 Analytical, 4 × 250 mm Dionex IonPac AG20 Guard, 4 × 50 mm
Flow:	1.0 mL/min
Column Temp.:	30 °C
Injection Volume:	25 µL
InGuard:	HRP, 9 × 24 mm
Concentrator:	Dionex IonPac UTAC-LP1, 4 × 35 mm
Eluent Source:	EGC II KOH with CR-ATC
Gradient:	Time (min) Eluent Conc. (mM) -20 50 -7.1 50 -7.0 7 -5.0 7 0.0 7 25.0 7 25.1 50
Detection:	Suppressed conductivity, Dionex ASRS 300 suppressor, 4 mm with external water mode, current 125 mA
Sample:	A. Sample #1 B. Spiked Sample #1

Peaks:	Conc. (mg/L) A	B
1. Nitrite	ND	0.016
2. Nitrate	0.084	0.130

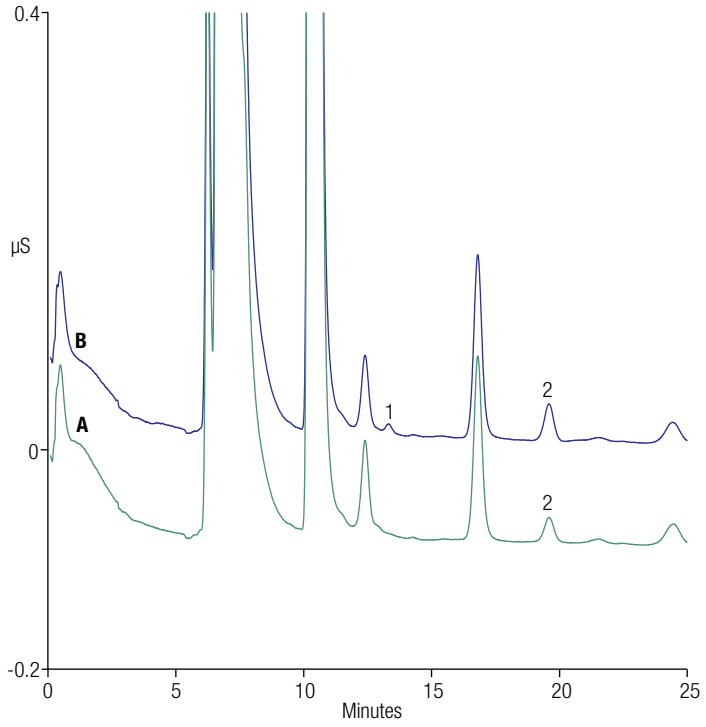
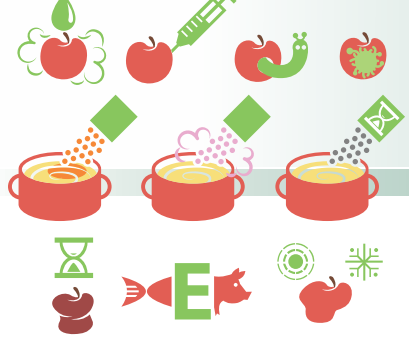


Figure 8-66. Overlay of chromatograms of Milk Sample #2 and Spiked Milk Sample #2.

Download Application Note 279: Time Savings and Improved Reproducibility of Nitrate and Nitrite Ion Chromatography Determination in Milk Samples



Nitrate and Nitrite in Drinking Water

The ion chromatographic determination of nitrite and nitrate in drinking water can be accomplished using direct UV detection of the analytes. The method is free from most ionic interferences due to the specificity of UV detection. The method is applicable to all drinking water samples. Bromide may also be separated from other ions detected using this method.

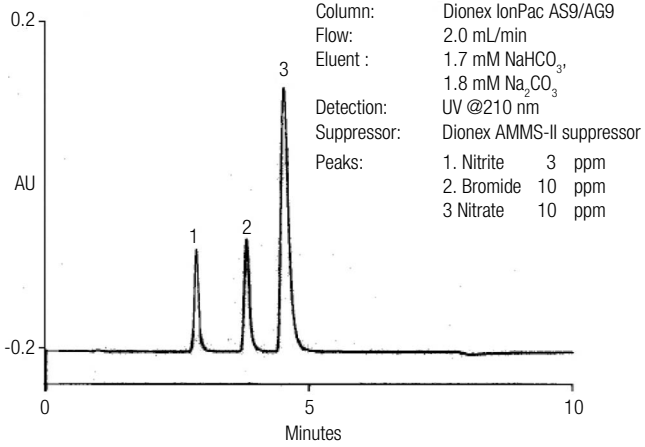
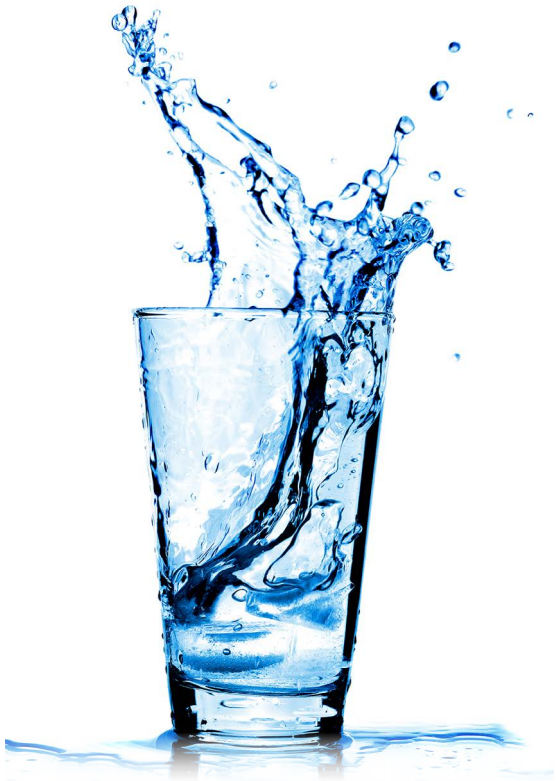
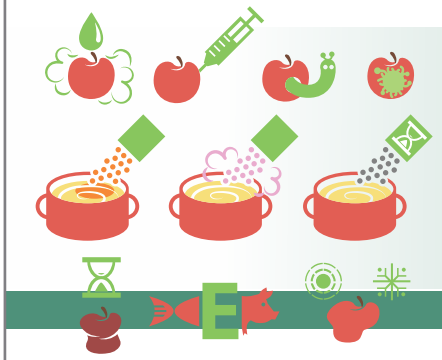


Figure 8-67. Direct UV detection of nitrite and nitrate in drinking water (preserved with sulfuric acid) with chemical suppression of eluent.



Download Application Update 132: Determination of Nitrite and Nitrate in Drinking Water Using Ion Chromatography with Direct UV Detection



Oxyhalides and Bromide in Water

To ensure that drinking water is safe for human consumption, it must be disinfected. Disinfection with either chlorine dioxide and/or ozone can result in the formation of oxyhalides such as chlorite, chlorate, and bromate. There are regulations regarding the concentrations of those three anions in drinking water in nearly all countries. The concentration of bromide is also of interest as it is a precursor of bromate, which is formed during ozonation.

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Oxyhalides and Bromide in Bottled Water

Unlike tap water, bottled water is treated as a food product in the U.S. and therefore regulated by the U.S. Food and Drug Administration (FDA). Bottled water must be disinfected to remove pathogenic organisms and ensure it is safe for human consumption. Ozone is favored by bottlers because it does not remain in the water and leaves no taste, but it does react with naturally occurring bromide to produce bromate, a suspected carcinogen. Chlorination of drinking water can produce trihalomethanes, haloacetic acids, and chlorate. While chlorine dioxide treatment generates inorganic oxyhalide DBPs, chlorite, and chlorate, and the presence of chloramine has been associated with the production of chlorate.

Bottled water is an increasingly popular product in the U.S. The FDA adopted the EPA's MCLs for chlorite and bromate and the analytical methods used to monitor these contaminants in public drinking water. The FDA also requires that bottled water manufacturers monitor their finished product for these contaminants at least once each year under current good manufacturing practice as stated in part 129 of the Code of Federal Regulations (21 CFR part 129).

Columns:	Dionex IonPac AG19 and AS19, 4 mm	Peaks A:	2. Bromate	9.2	µg/L
			3. Chlorate	375.0	
Flow:	1 mL/min		4. Bromide	2.5	
Temperature:	30 °C	Peaks B.	1. Chlorite	20.0	µg/L
Injection Volume:	250 µL		2. Bromate	19.5	
Eluent:	10 mM KOH 0–10 min, 10–45 mM 10–25 min		3. Chlorate	520.0	
			4. Bromide	22.5	
Eluent Source:	Dionex ICS-2000 EG with CR-ATC				
Detection:	Dionex ASRS ULTRA II, 4 mm recycle mode, 130 mA				

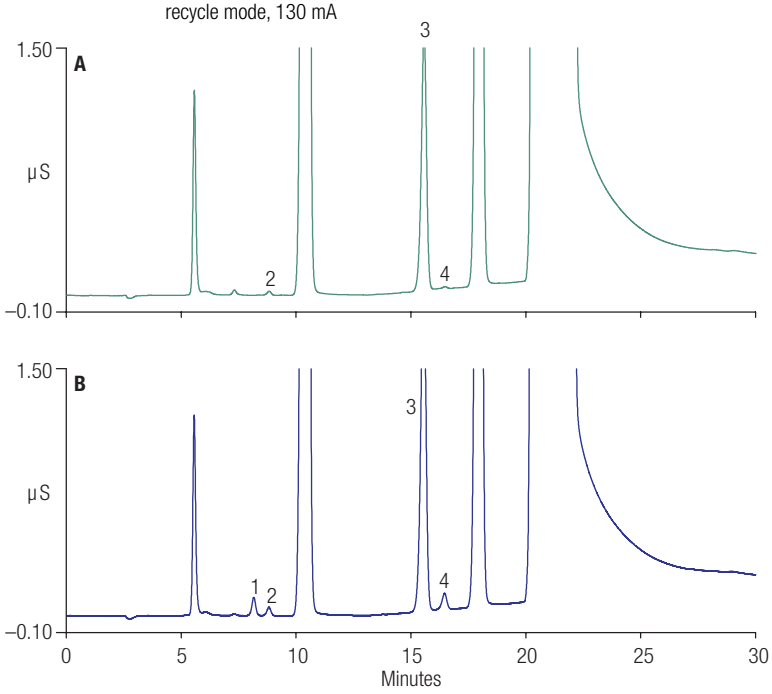
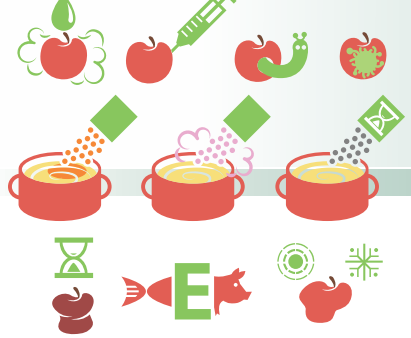


Figure 8-68. Determination of DBP anions and bromide in (A) bottled water 6 and (B) spiked bottled water 6 using the Dionex IonPac AS19 column.

Download Application Note 167: Determination of Trace Concentrations of Oxyhalides and Bromide in Municipal and Bottled Waters Using a Hydroxide-Selective Column with an RFIC System



Oxyhalides and Bromide in Drinking Water

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Download Application Note 136: 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

Download Application Note 149: Determination of Chlorite, Bromate, Bromide and Chlorate in Drinking Water by IC with an On-Line-Generated Postcolumn Reagent for Sub-µg/L Bromate Analysis

Download Application Note 168: Determination of Trace Concentrations of Disinfection By-Product Anions and Bromide in Drinking Water Using Reagent-Free IC Followed by Postcolumn Addition of o-Dianisidine for Trace Bromate Analysis

Download Application Note 184: Determination of Trace Concentrations of Chlorite, Bromate, and Chlorate in Bottled Natural Mineral Waters

Download Application Note 187: Determination of Sub-µg/L Bromate in Municipal and Natural Mineral Waters Using Preconcentration with Two-Dimensional IC and Suppressed Conductivity Detection

Download Application Note 208: Determination of Bromate in Bottled Mineral Water Using the CRD 300Carbonate Removal Device

Download Application Note 217: Determination of Haloacetic Acids in Water using IC-ESI-MS/MS

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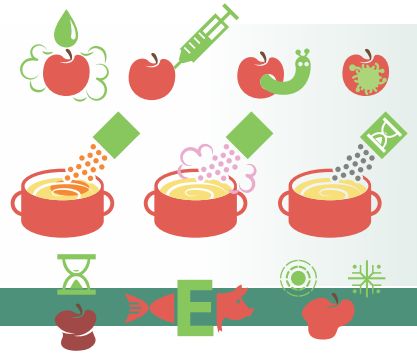

Patulin

Patulin is a mycotoxin found in moldy apples. While no tolerance level has been fixed for this substance, it is used as an indicator of quality in processed apple products. Hydroxymethylfurfural (HMF) is a product of thermal decomposition of sugars, and is used as an indicator of heat damage in processing of sweet foods.

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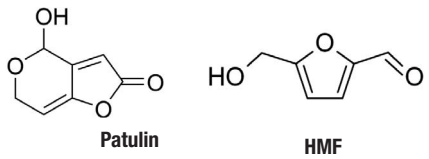
Patulin and Hydroxymethylfurfural in Apple Juice

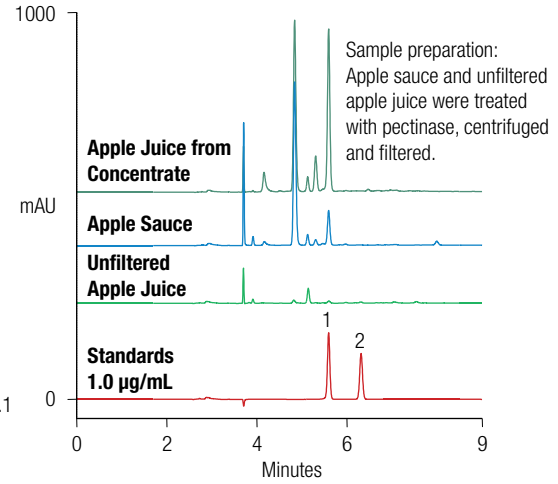
Both patulin and hydroxymethylfurfural are weakly hydrophobic, neutral compounds, and co-elute on many reversed-phase columns. Fruit juice is a complex matrix, so some form of sample cleanup is necessary. The traditional sample preparation involves off-line extraction using ethyl acetate which yields good recoveries for patulin, but not for HMF. In-line solid-phase extraction is expected to be more reproducible and involve less manual handling. The Acclaim Mixed-Mode WCX-1 permits organic acids and phenolics to wash out by ion exclusion well ahead of the HMF and patulin (which co-elute on this column). The auxiliary valve transfers the analytes to the Acclaim C30 column that provides excellent resolution of these two substances.

HPLC System:	UltiMate 3000 RSLC system ×2 dual gradient
Analytical Column:	Acclaim C30 3 µm
Dimension:	2.1 × 150 mm
SPE Column:	Acclaim Mixed-Mode WCX-1
Dimension:	3.0 × 50 mm
Flow:	Right: 0.40 mL/min, left: 0.40 mL/min
Temperature:	25 °C
Injection Volume:	60 µL
Mobile Phase:	Left pump A: Acetonitrile Left pump B: 1.0 mM dibasic sodium phosphate, 4.0 mM monobasic sodium phosphate, 0.1 mM tetrabasic sodium pyrophosphate; pH 6.5 Right pump A: Acetonitrile Right pump B: Water Right pump C: 12.5 mM ammonium formate, 50 mM formic acid, pH 3.1

Gradient Times (min):	-5.0	0.0	1.6	1.7	2.4	7.0	7.1	9.0
Left pump %A:	0.0	0.0	0.0	50.0		50.0	0.0	
Left pump %B:	100.0	100.9	100.0	50.0		50.0	100.0	
Right pump %A:	4.0	4.0	4.0			10.0	30.0	30.0
Right pump %B:	86.0	86.0	86.0			80.0	60.0	60.0
Right pump %C:	10.0	10.0	10.0			10.0	10.0	10.0
Aux. Valve:	Load		inject		load			

Aux. Valve:	10-port, 2-position configured for forward elution of SPE
Detection:	Diode Array, UV at 276 nm, 5 Hz, 1.0 s resp. time
Peaks:	1. Hydroxymethylfurfural (HMF) 2. Patulin





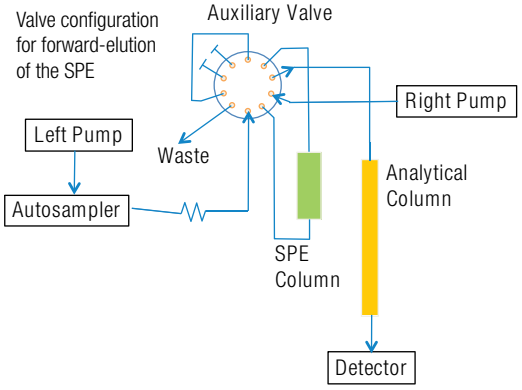
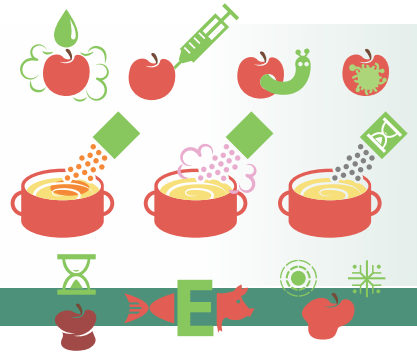
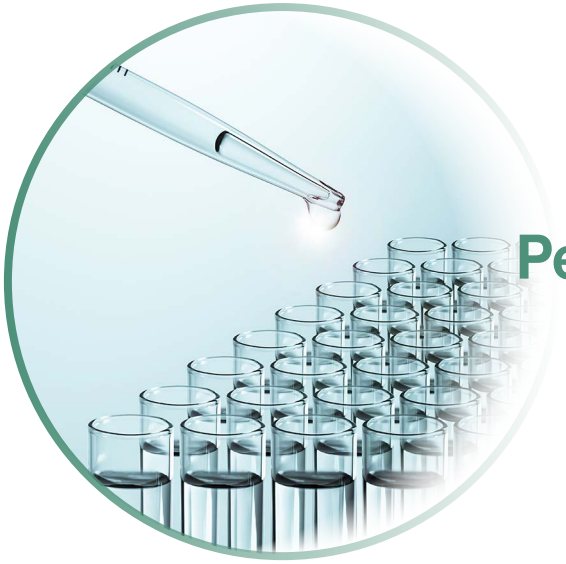


Figure 8-69. Patulin and hydroxymethylfurfural in apple juice using in-line SPE cleanup and concentration.





Perchlorate

Perchlorate, while naturally occurring, is often an environmental contaminant in areas where munitions, perchlorate salts, and highway flares are or have been manufactured. Perchlorate can replace iodide in the thyroid and that may lead to a variety of human health issues. Concern about the presence of perchlorate in drinking water has resulted in its being added to the US EPA Unregulated Contaminant Candidates Monitoring list and its concentration being regulated in a number of US states.

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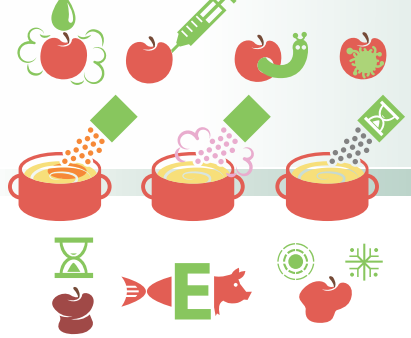


Perchlorate in Foods

Perchlorate is found in nitrate fertilizers, and is used as an ingredient for solid rocket propellant, explosives, and industrial processes like rubber manufacturing. This contaminant interferes with the iodide uptake into the thyroid gland, and can disrupt neurological development in fetuses and children.

Perchlorate in irrigation water can build up in a variety of crops, such as lettuce, spinach, melons, and grains. Sample preparation for perchlorate analysis of crops typically involves high speed blending and ultrasonication extraction, but these techniques are not efficient enough to extract tightly bound ions, such as perchlorate, from complex vegetation or other biosolid matrices. Additional cleanup steps, such as SPE, are also usually required.

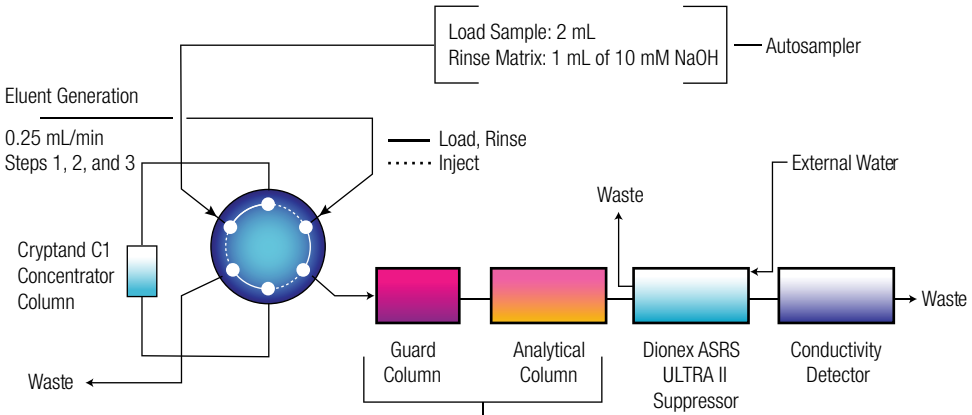
Minimum detection limits using a Dionex IonPac AS16 column and suppressed conductivity detection are <2.0 µg/kg for perchlorate extracted from spinach, melon, and corn.

Chromatographic Conditions

Columns:	Dionex IonPac AS16 Analytical, 2 × 250 mm Dionex IonPac AG16 Guard, 2 × 50 mm Dionex IonPac Cryptand C1 Concentrator, 4 × 35 mm
Eluent:	0.50, 65, and 100 mM NaOH
Backpressure:	2300 psi
Detection:	Dionex ASRS ULTRA II suppressor, external water mode, 100 mA current
Run Time:	46 min

Accelerated Solvent Extraction Conditions for Perchlorate

Extraction Solvent:	Water
Pressure:	1500 psi
Temperature:	80 °C
Equilibration Time:	5 min
Extraction Time:	5 min (static)
Solvent Flush:	30% (of cell volume)
Nitrogen Purge:	120 s (after extraction)
Extraction Cycles:	3
Cell Sizes:	33 mL and 100 mL

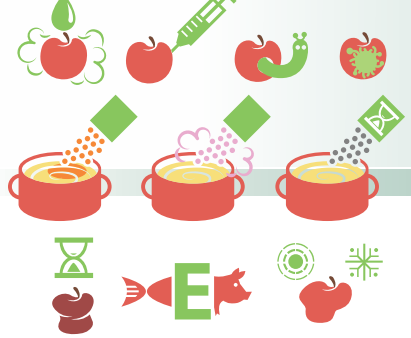


NaOH Eluent Generation

Step	Function	Conc.	Time
1	Perchlorate Transfer	0.5 mM	12 min
2	Analysis	65 mM	16 min
3	Column Cleanup	100 mM	2 min

Figure 8-70. The three steps for sodium hydroxide generation.

Download the Poster Note: Determination of Perchlorate Levels in Food and Soil Samples Using Accelerated Solvent Extraction and Ion Chromatography



Perchlorate in Foods

Column: Dionex IonPac AS16 Analytical, 2 × 250 mm
Dionex IonPac AG16 Guard, 2 × 50 mm
Dionex IonPac Cryptand CI Concentrator, 4 × 35 mm
Flow: 0.25 mL/min
Temperature: 35 °C
Eluent: 0.50, 65, and 100 mM sodium hydroxide
Detection: Suppressed conductivity, Dionex ASRS ULTRA, external water mode
Peak: 1. Perchlorate 50 ng/g

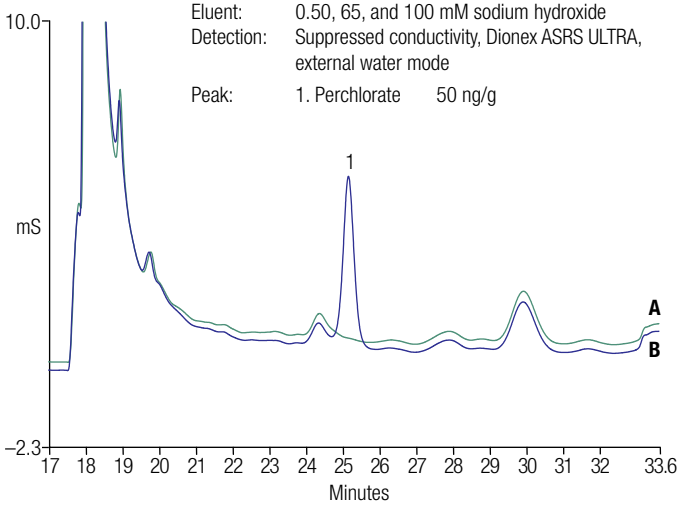


Figure 8-71. Chromatograms of (A) a melon "blank" obtained using accelerated solvent extraction, and (B) a 5 g melon sample spiked with perchlorate.

Column: Dionex IonPac AS16 Analytical, 2 × 250 mm
Dionex IonPac AG16 Guard, 2 × 50 mm
Dionex IonPac Cryptand C1 Concentrator, 4 × 35 mm
Flow: 0.25 mL/min
Temperature: 35 °C
Eluent: 0.50, 65, and 100 mM sodium hydroxide
Detection: Suppressed conductivity, Dionex ASRS ULTRA, external water mode
Peak: 1. Perchlorate 10 ng/g

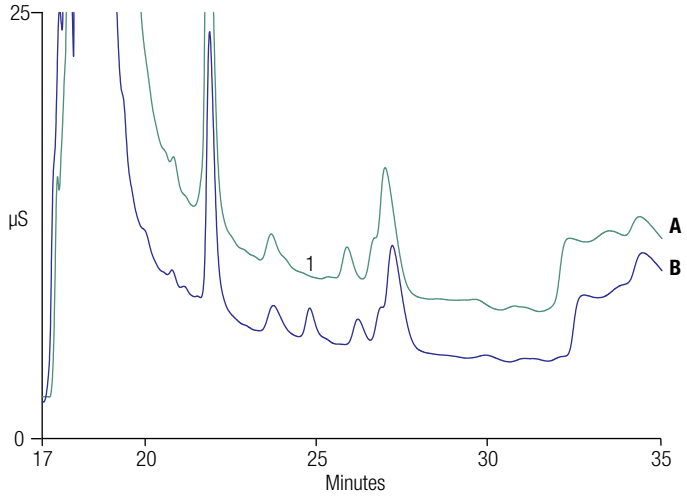


Figure 8-72. Chromatograms of (A) a spinach "blank" obtained using accelerated solvent extraction, and (B) a 5 g spinach sample spiked with perchlorate.

Table 8-9.

Matrix	Avg. Recovery (%, n = 21)	*MDL (µg/kg)	*RQL (µg/kg)
Melon	103.3	0.72	2.9
Corn	96.3	1.4	5.6
Spinach	101.6	2.0	8.0

*Analysis was performed using EPA Method 314.1 with a Dionex ICS-2500 ion chromatography system.

Download the Poster Note: Determination of Perchlorate Levels in Food and Soil Samples Using Accelerated Solvent Extraction and Ion Chromatography

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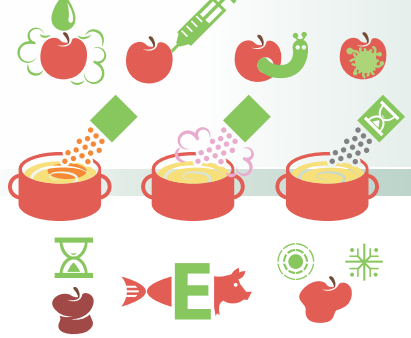


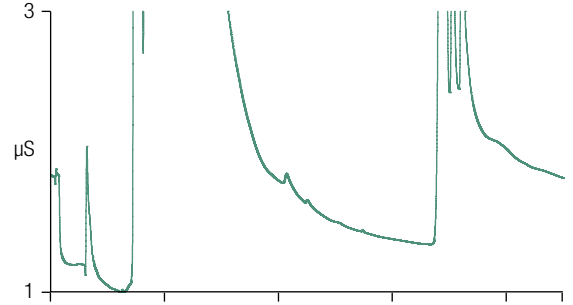
Perchlorate in Drinking Water

In 2005 the EPA published Method 314.1 as an update to Method 314.0 to improve the sensitivity for perchlorate in high-ionic-strength matrices. This method requires the concentration of a 2 mL sample on a Dionex IonPac Cryptand C1 preconcentration column followed by matrix elimination with 1 mL of 10 mM sodium hydroxide. Perchlorate is then separated by using a 2 mm Dionex IonPac AS16 column in the primary method. If perchlorate is positively identified with this method, then the sample must be reanalyzed on a confirmatory column, the Dionex IonPac AS20, to verify the presence of perchlorate and thereby reduce the likelihood of a false positive.

Alternatively, EPA Method 314.2, a two-dimensional ion chromatographic approach can be used to resolve perchlorate from high concentrations of common matrix ions. The first dimension uses a 4 mm Dionex IonPac AS20 column to divert the matrix ions while 5 mL of the suppressed effluent containing perchlorate is trapped on a Dionex IonPac TAC-ULP1 Trace Anion Concentrator Column and then separated on a 2 mm Dionex IonPac AS16 column in the second dimension for quantitative analysis. This method provides several advantages, such as the ability to inject large sample volumes, the ability to focus the perchlorate that is partially resolved in the first dimension onto a concentrator column and separate it in the second dimension, and the ability to combine two different column chemistries to enhance the selectivity and reduce the possibility of a false positive. Application Note 178 demonstrates this approach for determining trace concentrations of perchlorate in water samples using the same criteria specified in Method 314.1.

A. First Dimension

Column:	Dionex IonPac AG20, AS20, 4 mm
Flow:	1 mL/min
Temperature:	30 °C
Injection Volume:	4,000 µL
Eluent:	35 mM KOH 0–30 min, step to 60 mM at 30.1 min, 60 mM 30.1–40 min; step to 35 mM at 40.1 min, 35 mM 40.1–45 min
Eluent Source:	Dionex ICS-3000 EG
Detection:	Dionex ASRS ULTRA II suppressor, 4 mm, auto-suppression, external water mode



B. Second Dimension

Column:	Dionex IonPac AG16, AS16, 2 mm
Eluent:	65 mM KOH
Eluent Source:	IDionex CS-3000 EG
Temperature:	30 °C
Flow Rate:	0.25 mL/min
Injection Volume:	5 mL
Concentrator:	Dionex TAC-ULP1, 5 × 23 mm
Detection:	Dionex ASRS ULTRA II suppressor, 2 mm, external water mode
Peaks:	1. Perchlorate 0.5 µg/L

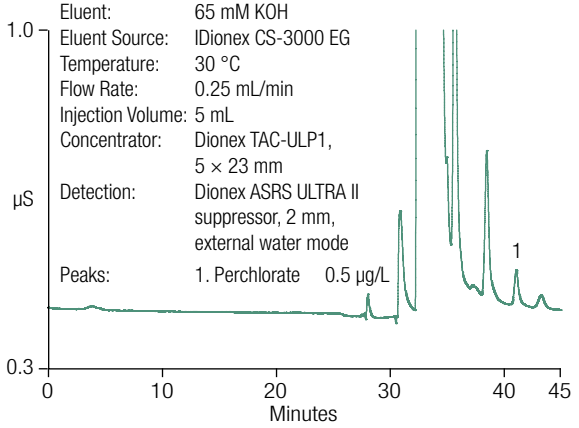
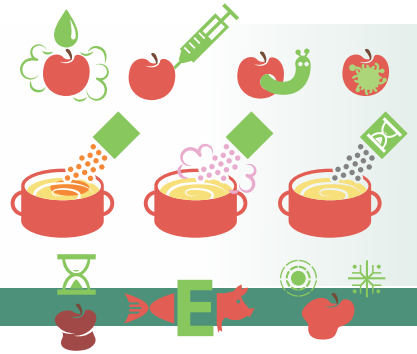


Figure 8-73. Chromatogram of drinking water D fortified with 0.5 µg/L perchlorate in the (A) first dimension and (B) second dimension.

Download Application Note 178: Improved Determination of Trace Concentrations of Perchlorate in Drinking Water Using Preconcentration with Two-Dimensional Ion Chromatography and Suppressed Conductivity Detection



Phenylurea Compounds

Phenylurea compounds are widely used as agricultural pesticides. Due to their slow degradation, they are frequently detected in surface waters at concentrations above 0.1 mg/L, which is higher than the European Commission's drinking water limit often used as a quality standard for natural water.

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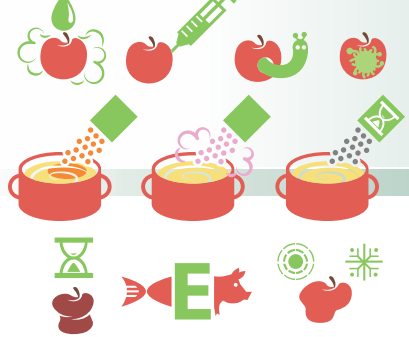

Phenylurea Compounds

U.S. EPA Method 532.3 the method typically used for the sensitive determination of phenylurea compounds, uses reversed-phase high performance liquid chromatography (RP-HPLC) with UV detection.

This application presents an efficient HPLC method for the sensitive determination of nine phenylurea compounds in drinking water samples using on-line solid-phase extraction (SPE) and UV detection with method detection limits (MDLs) that meet those reported in U.S. EPA Method 532 and concentration limits set in the European Commission's Council Directive 98/83/EC.

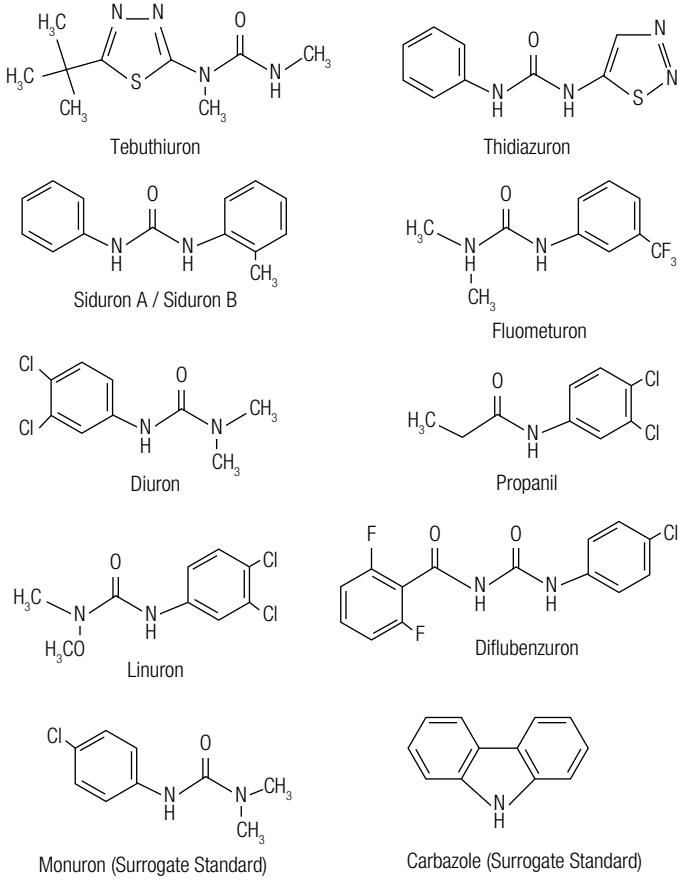

Figure 8-74. Structures of phenylurea compounds listed in U.S. EPA Method 532 and their surrogate standards.

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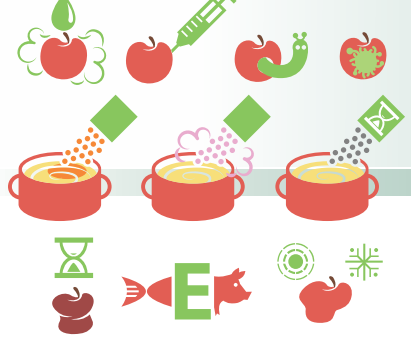

Phenylurea Compounds

For On-Line SPE

Cartridge: Dionex SolEx HRP, 12–14 µm, 2.1 × 20 mm (Use V-3 Cartridge Holder)
Flow: 1.0 mL/min
Injection Volume: 2500 µL on the on-line SPE cartridge
Mobile Phase: A: H_2O, B: methanol
Gradient: 0–4 min, 10–100% B; 13 min, 100% B; 13.1–20 min, 10% B

For Separation

Column: Acclaim 120 C18, 3 µm Analytical, 3.0 × 150 mm
Flow: 0.6 mL/min
Temperature: 25 °C
Mobile Phase: A: 20 mM $HCOONH_4$, B: acetonitrile
Gradient: 0–4 min, 35% B; 4.1 min, 40% B; 7.5–15.8 min, 60% B; 16 min, 35% B
Detection: UV absorbance at 245 nm

Peaks: 1. Tebuthiuron 5.0 µg/L each
2. Thidiazuron
3. Monuron (Surrogate Standard, 20 µg/L)
4. Fluometuron
5. Diuron
6. Propanil
7. Siduron A
8. Siduron B
9. Linuron
10. Carbazole (Surrogate Standard, 20 µg/L)
11. Diflubenzuron

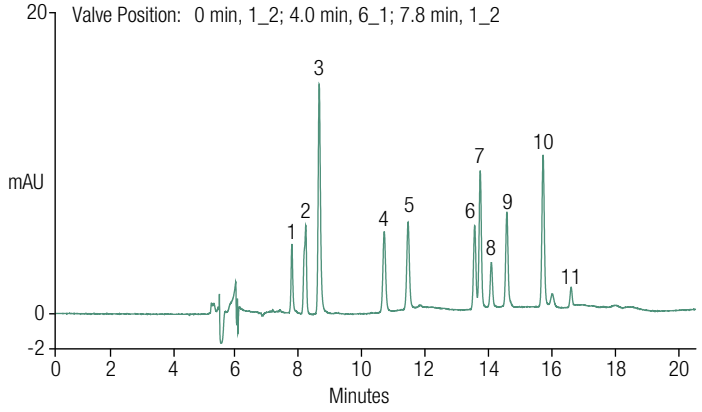

Figure 8-75. Chromatogram of phenylurea compounds and surrogate standards

See Figure 8-66 for Conditions for On-Line SPE and Separation

Samples: A. Green tea
B. Green tea (already 3-fold dilution with water) fortified with phenylurea standards (2.5 µg/L each)
C. Mixture of phenylurea standards (2.5 µg/L each).

Peaks: 1. Tebuthiuron 5.0 µg/L each
2. Thidiazuron
3. Monuron (Surrogate Standard, 20 µg/L)
4. Fluometuron
5. Diuron
6. Propanil
7. Siduron A
8. Siduron B
9. Linuron
10. Carbazole (Surrogate Standard, 20 µg/L)
11. Diflubenzuron

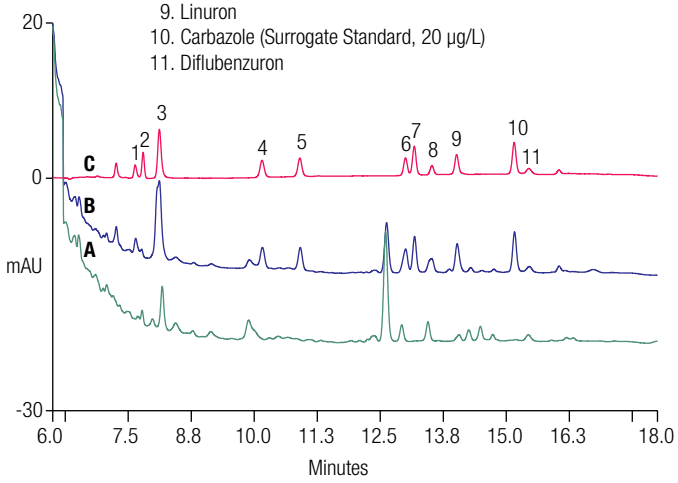

Figure 8-76. Chromatograms of a green tea sample, the same sample fortified with phenylurea standards, and a mixture of phenylurea standards.

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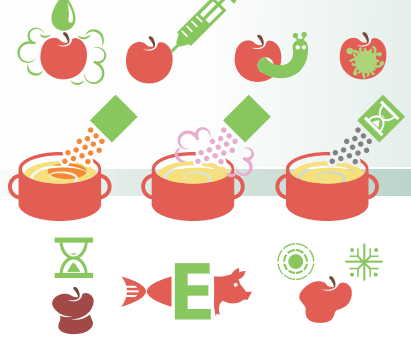

Phenylurea Compounds

See Figure 8-66 for Conditions for On-Line SPE and Separation

Samples: A. tap water
B. tap water fortified with phenylurea standards (2.5 µg/L each)

Peaks:

1.	Tebuthiuron	5.0 µg/L each
2.	Thidiazuron	
3.	Monuron (Surrogate Standard, 20 µg/L)	
4.	Fluometuron	
5.	Diuron	
6.	Propanil	
7.	Siduron A	
8.	Siduron B	
9.	Linuron	
10.	Carbazole (Surrogate Standard, 20 µg/L)	
11.	Diflubenzuron	

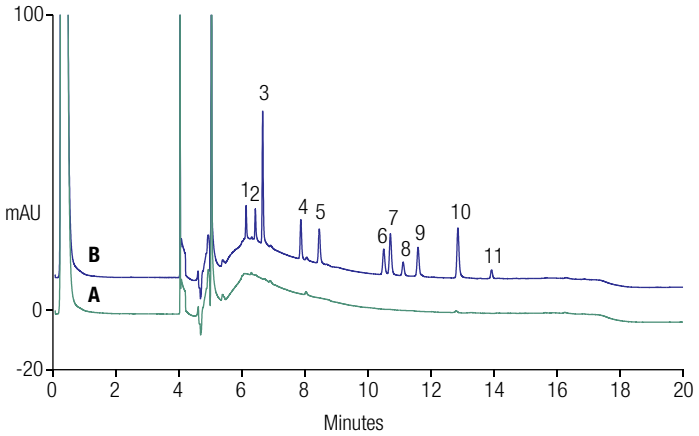

Figure 8-77. Chromatograms of a tap water sample, and the same sample fortified with phenylurea standards.

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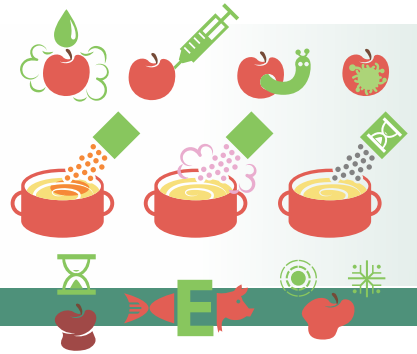

Phthalates

Phthalates are a class of chemical compounds widely used as plasticizers for polyvinyl chloride resins, adhesives, and cellulose film coating. To date nearly 20 kinds of phthalates have been used for these purposes. Phthalates are potentially hazardous to human health—especially to children's health—due to their classification as endocrine disruptors. This has resulted in regulations regarding the types and levels of phthalates allowable in plastic toys, water containers, textiles, and foods.

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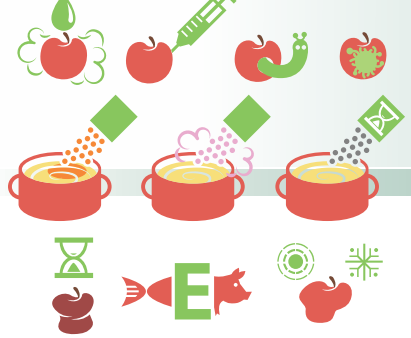


Phthalates

Application Note 1045 describes an HPLC-UV method that can separate all the phthalates listed in the regulated methods.

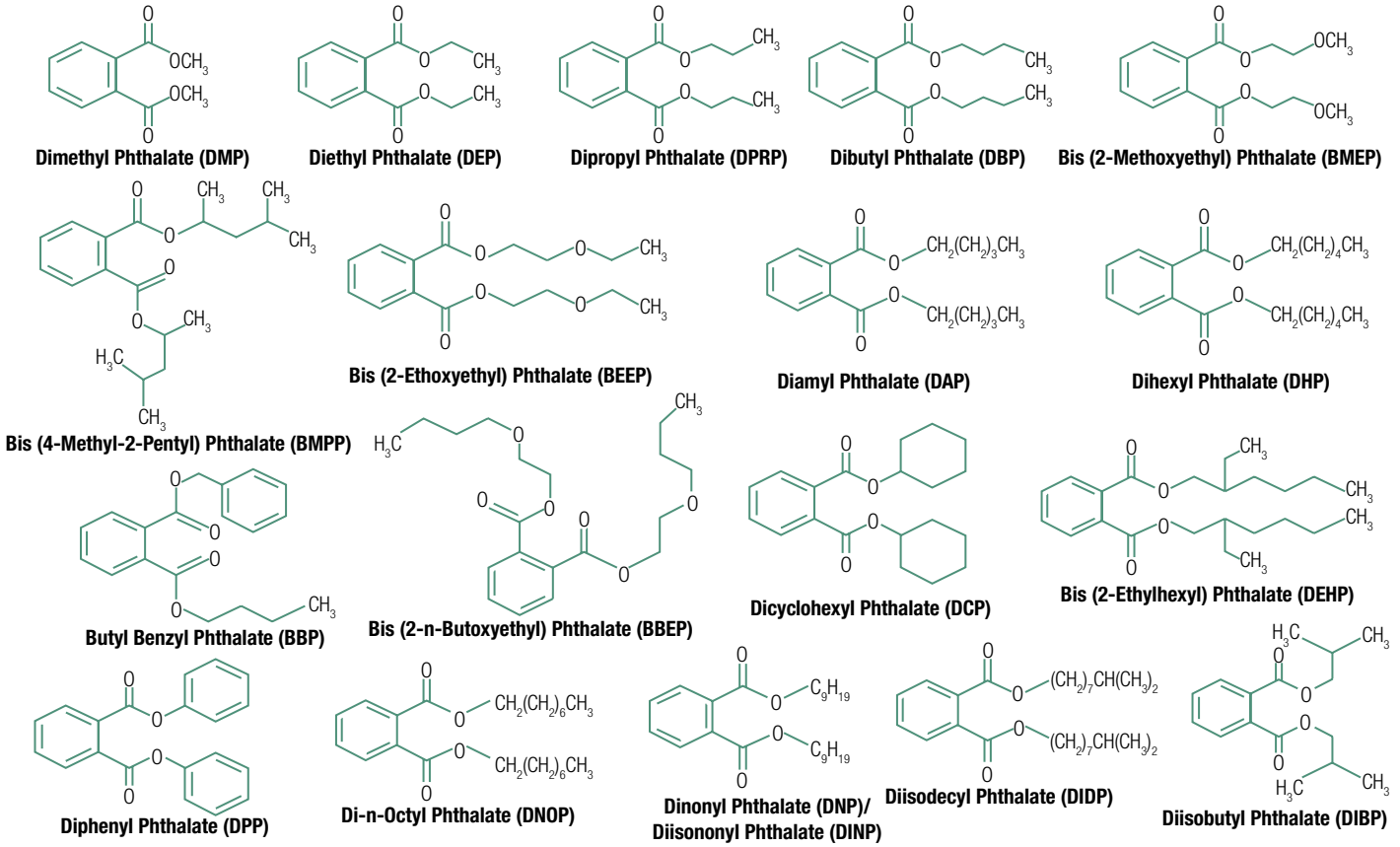
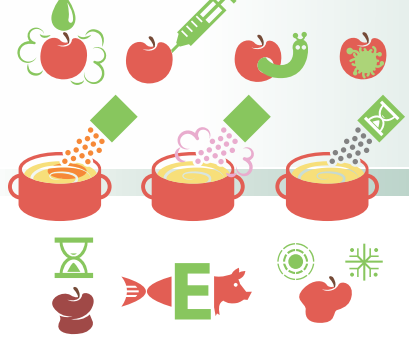


Figure 8-78. Structures of 19 phthalates (isomers DNP and DINP have the same structure).



Phthalates

Column:	Acclaim C30, 3 µm, 3.0 × 150 mm
Flow:	1.0 mL/min
Temperature:	45 °C
Injection Volume:	5 µL
Mobile Phase:	A: Water B: CH_3CN C: CH_3OH
Gradient:	0 min, B: 35%, C: 0%, curve 5; 12–22 min, B: 25–100%, C: 45–0%; 22.5–25 min, B: 35%, C: 0%, curve 5
Detection:	UV absorbance at 228 nm
Chromatograms:	A. Drinking Water Sample #1 B. A sample spiked with a phthalate mixed standard

Peaks (5 µg/mL each):

1. DMP	2. BMEP	3. DEP
4. BEEP	5. DPP	6. BBP
7. DIBP	8. DBP	9. BBEP
10. DAP	11. DCP	12. BMPP
13. DHP	14. DEHP	15. DNOP
16. DNP	17. DPRP	

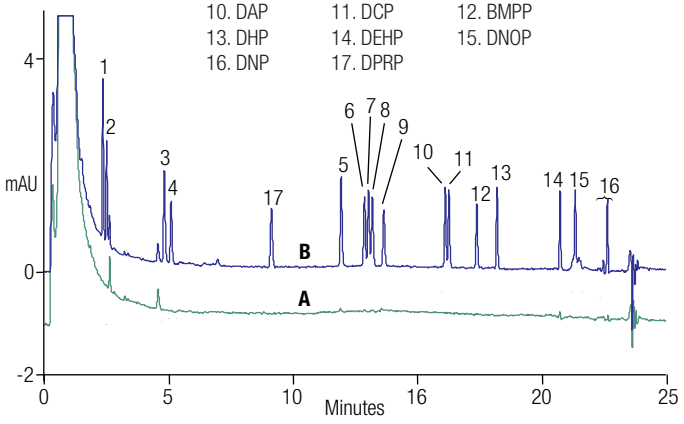


Figure 8-79. Blank-subtracted chromatograms of a drinking water sample and the same sample spiked with a phthalate mixed standard using an Acclaim C30 column.

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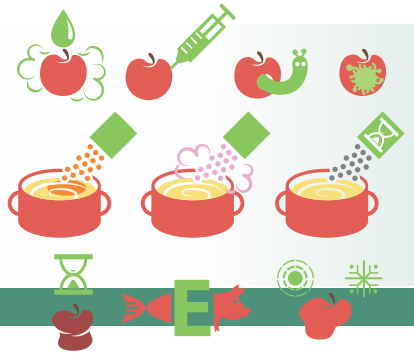

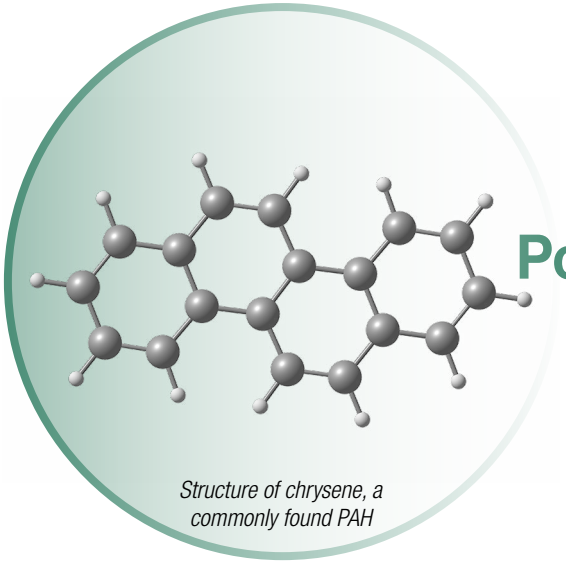

Structure of chrysene, a commonly found PAH

Polycyclic Aromatic Hydrocarbons

Numerous polycyclic aromatic hydrocarbons (PAHs) are carcinogenic, making their presence in foods and the environment a health concern. Regulations around the world limit levels of a variety of PAHs in drinking water, food additives, cosmetics, workplaces, and factory emissions.

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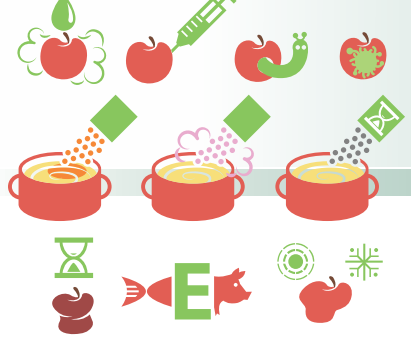


Polycyclic Aromatic Hydrocarbons

PAHs have traditionally been separated using HPLC, but method detection limits (MDLs) of HPLC techniques employing direct injection of samples are too high for the detection of the low concentrations in real samples that are near the regulated limit. Therefore, the analytes in these samples require preconcentration before analysis.

The U.S. EPA prescribes liquid-liquid extraction and liquid-solid extraction (also called solid-phase extraction, SPE) methods for pre-concentrating PAHs in drinking water samples. However, preparing individual samples is time consuming for each of the two extraction methods, and a new SPE cartridge must be used for each sample when using the SPE method. The expense of using multiple SPE cartridges and the associated manual labor can be eliminated with online SPE combined with the subsequent HPLC analysis. This technique delivers a simple, rapid, and accurate means for determining PAHs at low concentrations in water samples.

Application Note 213 describes the use of online SPE followed by HPLC with fluorescence or UV detection for the measurement of numerous PAHs in drinking water.

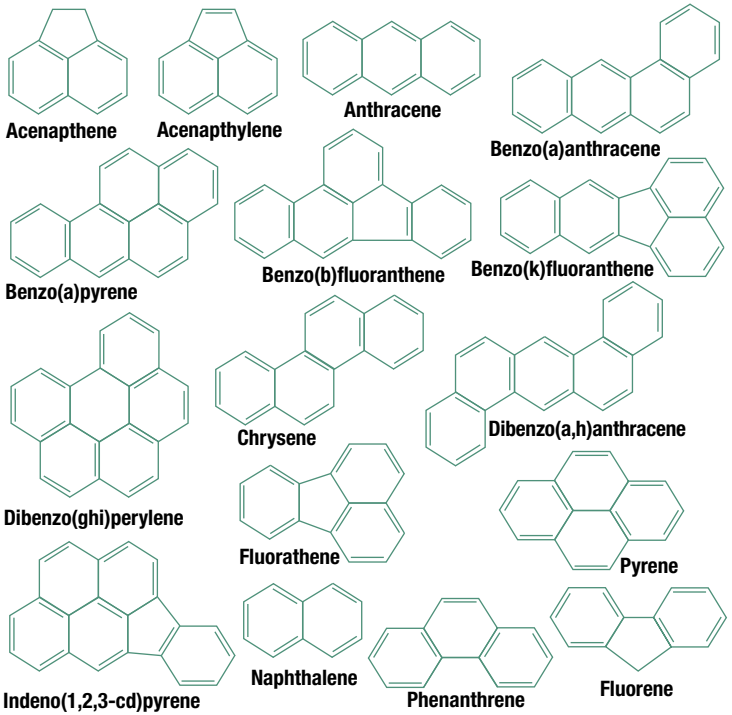


Figure 8-80. Structures of the 16 PAHs specified in U.S. EPA Method 550.1.

Download Application Note 213: Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in Tap Water Using On-Line Solid-Phase Extraction Followed by HPLC with UV and Fluorescence Detections

Polycyclic Aromatic Hydrocarbons

PAHs in Tap Water

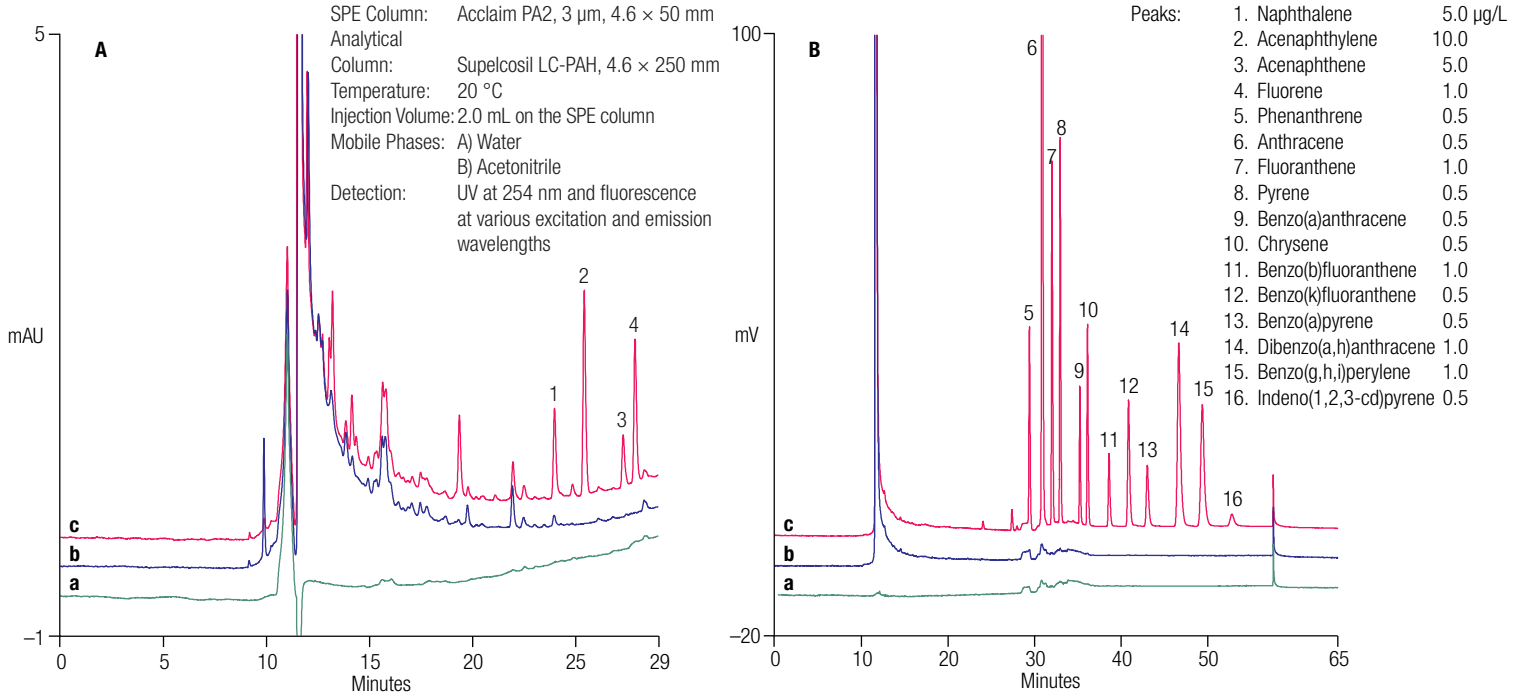
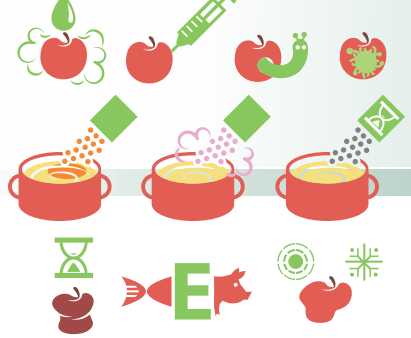


Figure 8-81. Chromatograms obtained by A) UV at 254 nm and B) FL at different wavelengths. Chromatograms of (a) blank, (b) tap water, and (c) tap water spiked with a PAH standard mixture.



Polycyclic Aromatic Hydrocarbons

PAHs in Edible Oils

PAHs also occur in charbroiled and dried foods, and may form in edible oils by pyrolytic processes, such as incomplete combustion of organic substances. PAHs in foods can also result from petrogenic contamination.

The European Commission regulates the amounts of PAHs in foods, and has imposed a limit of 2.0 µg/kg for benzo[a]pyrene (BaP) in edible oils, as BaP was determined to be a good indicator of PAH contamination.

On-Line SPE Column:	DACC, 3.0 × 80 mm
Analytical Columns:	Two PAH columns 4.6 × 250 mm for separation
Flow:	1 mL/min
Temperature:	30 °C for column, 40 °C for autosampler
Injection Volume:	80 µL
Eluent:	A) Water, B) Acetonitrile for both loading and analysis pumps C) Isopropanol for loading pump
Detection:	Fluorescence
Sample:	Mixture of PAHs standard

Peaks:	µg/kg
1. Phenanthrene	20
2. Anthracene	20
3. Fluoranthene	20
4. Pyrene	20
5. Benzo[a]anthracene	20
6. Chrysene	20
7. Benzo[b]fluoranthene	20
8. Benzo[k]fluoranthene	20
9. Benzo[a]pyrene	20
10. Dibenzo[a,h]anthracene	20
11. Benzo[g,h,i]perylene	20
12. Indeno[1,2,3-cd]pyrene	20
13. Benzo[b]crysene (added as I.S.)	20

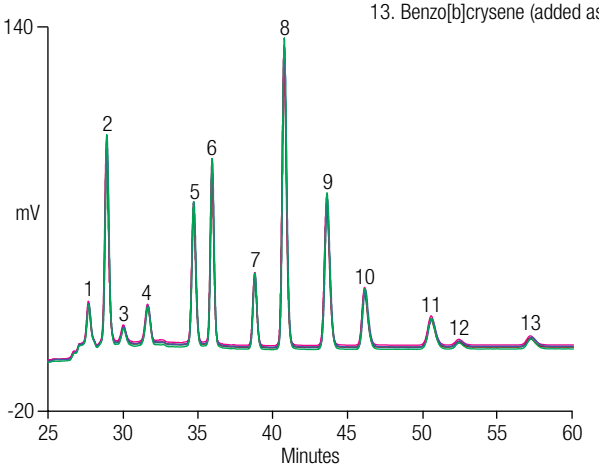


Figure 8-82. Overlay of chromatograms of seven serial injections of olive oil sample 1 spiked with a PAH standard mixture (20 µg/kg).

On-Line SPE Column:	DACC, 3.0 × 80 mm
Analytical Columns:	Two PAH columns 4.6 × 250 mm for separation
Flow:	1 mL/min
Temperature:	30 °C for column, 40 °C for autosampler
Injection Volume:	80 µL
Eluent:	A) Water, B) Acetonitrile for both loading and analysis pumps C) Isopropanol for loading pump
Detection:	Fluorescence

Peaks:
1. Phenanthrene
4. Pyrene
5. Benzo[a]anthracene
6. Chrysene
7. Benzo[b]fluoranthene
8. Benzo[k]fluoranthene
9. Benzo[a]pyrene
11. Benzo[g,h,i]perylene
12. Indeno[1,2,3-cd]pyrene

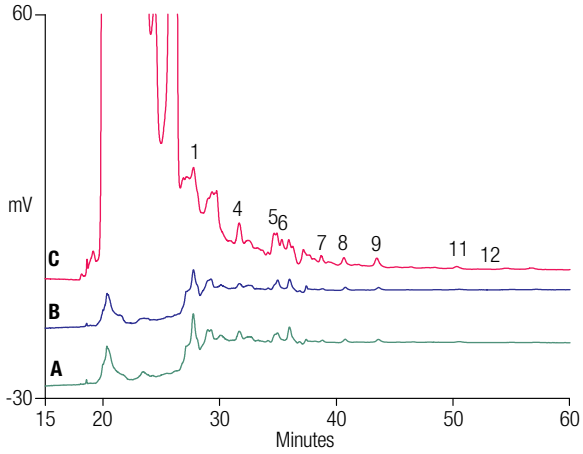
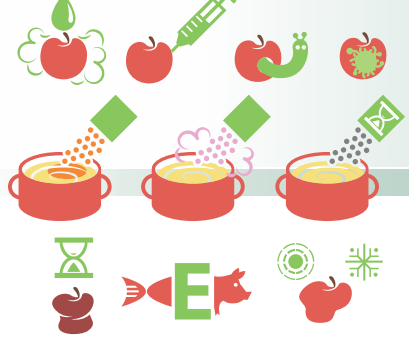


Figure 8-83. Overlay of chromatograms of A) olive oil 1, B) olive oil 2, and C) sesame oil samples.

Download Application Note 196: Determination of Polycyclic AromaticHydrocarbons (PAHs) in Edible Oils by Donor-Acceptor Complex Chromatography (DACC)-HPLC with Fluorescence Detection



Polycyclic Aromatic Hydrocarbons

PAHs in Tea

A challenging field of application is the determination of polycyclic aromatic hydrocarbon (PAH) contamination in foodstuffs, e.g., tea samples. After water, tea is the most widely consumed beverage in the world. While tea has the reputation of being healthy due to many pharmaceutically active ingredients and antioxidants, tea leaves also act as a perfect enrichment matrix for environmental pollutants. In particular, PAHs are a critical class of contaminants requiring careful and sensitive monitoring. Green, black, and oolong tea are all processed using a multistep procedure that exposes them to many sources for PAHs. Using the high-performance Thermo Scientific Dionex FLD-3100/3400RS Fluorescence Detector for UHPLC, and its ability to rapidly switch wavelengths, determination of PAHs in different tea samples was achieved with run times of less than 6 min, thus ensuring high sample throughput.

Column:	C18 PAH, 3 × 100 mm, 3 µm	Data Collection Rate:	100 Hz
Flow:	2.0 mL/min	Response Time:	0.02 s
Column Temp.:	30 °C	Lamp Mode:	Standard
Injection Volume:	2 µL	Photomultiplier Tube:	1 (FLD-3400RS)
Eluent:	A: Water		
	B: Acetonitrile		

Peaks: 1. Naphthalene
2. 1-Methylnaphthalene
3. 2-Methylnaphthalene
4. Acenaphthene
5. Fluorene
6. Phenanthrene
7. Anthracene
8. Fluoranthene
9. Pyrene
10. Benzo(a)anthracene
11. Chrysene
12. Benzo(b)fluoranthene
13. Benzo(k)fluoranthene
14. Benzo(a)pyrene
15. Dibenzo(a,h)anthracene
16. Benzo(g,h,i)perylene
17. Indeno(1,2,3-cd)pyrene

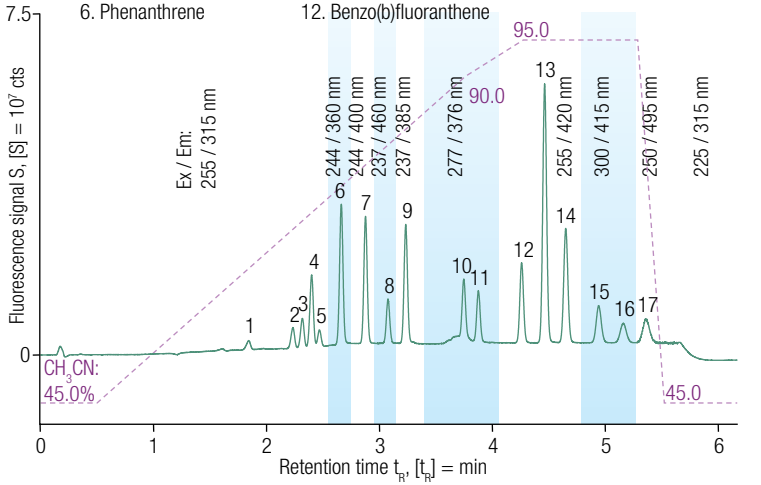


Figure 8-84. Separation of the 17 fluorescent PAHs of the EPA Method 610 standard mix; tints mark the dedicated detection parameters.

Polycyclic Aromatic Hydrocarbons

Column:	C18 PAH, 3 × 100 mm, 3 µm
Flow:	2.0 mL/min
Column Temp.:	30 °C
Injection Volume:	2 µL
Eluent:	A: Water B: Acetonitrile
Data Collection Rate:	100 Hz
Response Time:	0.02 s
Lamp Mode:	Standard
Photomultiplier Tube:	1 (FLD-3400RS)

Samples:
A. EPA-PAH 610 standard, 10 ng.mL-1
B. Black tea, St. Petersburg, solid-liquid extract
C. Black tea, St. Petersburg, tea liquor
D. Ahmad black tea, London, solid-liquid extract
E. Korean green tea, solid-liquid extract
F. Brazilian Mate tea, solid-liquid extract

Peaks:
1. Phenanthrene
2. Anthracene
3. Fluoranthene
4. Pyrene
5. Chrysene
6. Benzo(b)fluoranthene
7. Benzo(k)fluoranthene
8. Benzo(a)pyrene
9. Benzo(g,h,i)perylene
10. Indeno(1,2,3-cd)pyrene

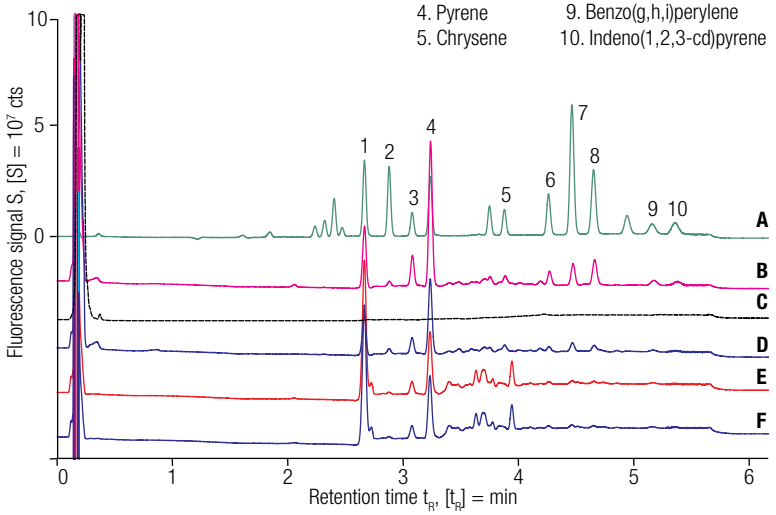
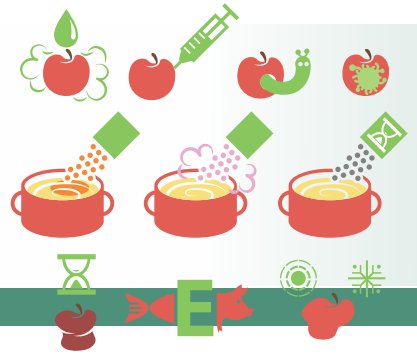
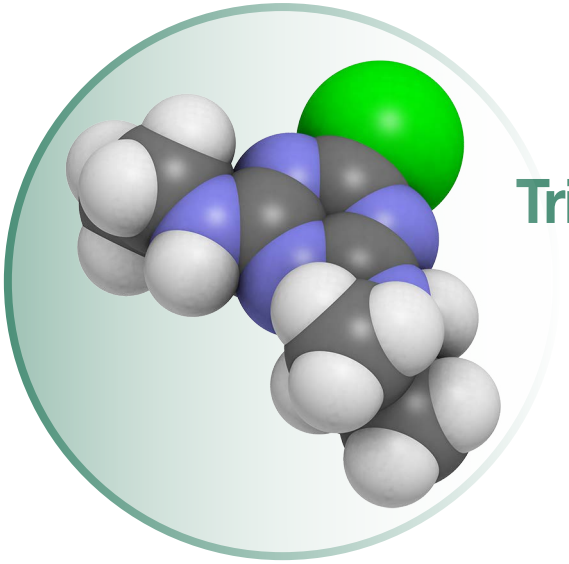


Figure 8-85. Separation of PAHs in tea samples.





Triazine Herbicides

Atrazine is a selective herbicide used for the control of weeds in crops such as asparagus, corn, sorghum, sugar cane, and pineapple. It is also used in forestry for non-selective weed control in non-crop areas. Today, it is the most widely used herbicide in the United States. As a result of widespread and long-term usage, atrazine and other triazine herbicide metabolites can be found at low levels in the environment and groundwater. Monitoring of atrazine, its metabolites desethyl-atrazine and desisopropylazine, and other triazine herbicides is important for environmental protection and food safety control.

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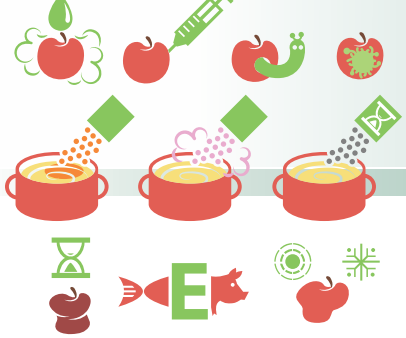

Triazine Herbicides

Triazine pesticides can be separated by HPLC using an Acclain 120 C18 column and an acetonitrile/ammonium acetate gradient.

Triazine herbicides are detected using ESI in positive mode.

Column:	Acclaim 120 C18, 5 µm
Flow:	0.25 mL/min
Temperature:	30 °C
Injection Volume:	10 µL
Dimensions:	2.1 × 100 mm
Mobile Phase:	35% Acetonitrile
	65% Ammonium acetate, pH 5
Detection:	MSQ MS
ESI:	Positive
Probe:	400 C
Needle:	2.5 kV
Cone Voltage:	Set per ion
Samples:	Seven herbicides at 1 ng on column

Peaks	m/z
1. Simazine	202
2. Atrazine	216
3. Prometon	226
4. Ametryn	228
5. Propazine	230
6. Prometryn	242
7. Terbutryn	242

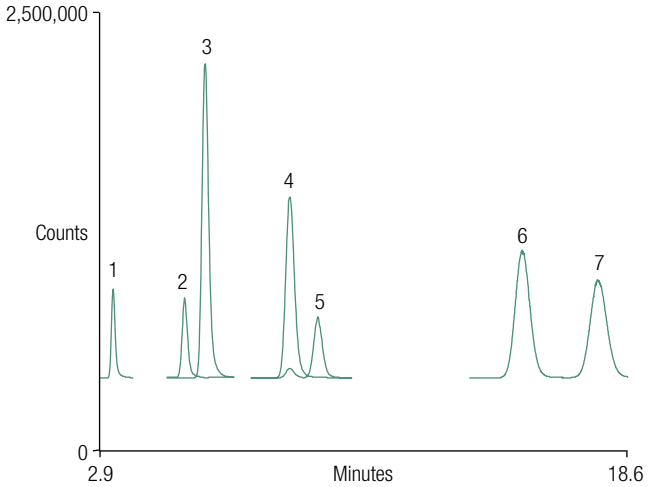

Figure 8-86. Sensitive detection of triazine herbicides on the Acclaim 120 C18 column with MS detection. Shown are seven simultaneous single-ion chromatograms optimized for positive identification.

Did You Know?

Triazine herbicides are photosystem II inhibitors. They reduce electron flow from water to $NADP^+$ during photosynthesis, ultimately resulting in plant death.

Download Application Note 453: UHPLC Separation of Triazine Herbicides at Elevated Temperature

Download Application Note ANCCSCETPEST: Analysis of Triazine Pesticides Using a Core Enhanced Technology Accucore HPLC Column

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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

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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

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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

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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

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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

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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

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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

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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

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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
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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

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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
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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

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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

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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

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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

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Product Number	Technique	Title
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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

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