



Accurate, reproducible anionic and cationic polar pesticide quantitation
One Thermo Scientific Dionex IC-MS/MS system



Expand analytical scope

Quantify anionic and cationic polar pesticides with one IC-MS/MS system

Expand the scope of your food and environmental sample testing to include multi-residue anionic and cationic polar pesticides. A Thermo Scientific™ ion chromatography tandem mass spectrometry (IC-MS/MS) system overcomes the challenges of achieving accurate and reproducible trace-level quantitation of ionic polar pesticides by eliminating time-consuming derivatization, minimizing “sticky” flow-path surfaces, and enhancing chromatographic resolution. With only a change of the eluent, column set, suppressor, and the trap column, it's easy to convert a Thermo Scientific IC-MS/MS system from anionic to cationic polar pesticides analysis, maximizing return on investment. What's more, with the Thermo Scientific™ Dionex™ ICS-6000 HPIC system, you can simultaneously run both anionic and cationic polar pesticide methods on single or multiple samples.



Eliminate derivatization:

Using ion exchange technology removes the need to derivatize hence saving time and reducing manual steps.

Cleaner samples:

The Quick Polar Pesticides (QuPPE) method helps to extract the pesticides of interest from food matrices before the chromatography.

Minimize analyte loss:

Some polar pesticides can stick, especially to glass and metal surfaces, making accuracy and reproducibility difficult to achieve, especially with quaternary ammonium pesticides like diquat and paraquat. Plastic vials and all-PEEK -flowpath reduce stickiness through the system, including columns.

Resolve challenging analytes:

Similar pesticide masses are difficult to chromatographically resolve using traditional LC columns, making their identification and accurate qualification difficult. Thermo Scientific™ Dionex™ columns are designed for ionic polar pesticides analysis, especially the Thermo Scientific™ Dionex™ CS21-fast-4µm column, which resolves quaternary amine cationic polar pesticides especially paraquat, and diquat.

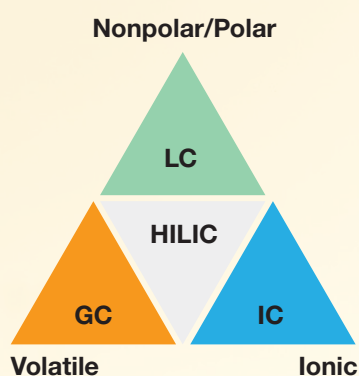
Expand analytical scope:

By swapping out a few consumables, you can analyze either anionic or cationic polar pesticides with a single IC instrument.

Address pesticide analysis challenges with IC-MS/MS

Pesticide analysis challenges

Maximum Residue Limits (MRLs) for pesticides on and in foods and in the environment have been established by regulatory authorities in most countries. Due to different toxicity levels and other factors such as environmental persistence, MRLs vary widely ranging from mg/kg (ppm) to µg/kg (ppb). Targeted quantitation of pesticides at these trace levels is challenging due to the complexity of food matrices and requirements for tedious sample preparation.



Chromatographic selectivity. IC columns provide complementary selectivity to RPLC and HILIC columns.

Gain more insight, increase confidence IC-MS/MS provides:

Adding MS detection increases confidence and dramatically improves the capabilities of an IC system. IC-MS/MS in particular maximizes your ability to detect and quantify co-eluting compounds and trace components.

IC-MS provides:

- Higher sensitivity and selectivity
- Increased resolution in complex matrices
- Accurate quantitation
- Mass confirmation of peaks, reducing false negatives and positives

IC-MS/MS advantages

Chromatography coupled with MS/MS is the standard for trace-level quantitation of target contaminants. IC is the technique of choice for polar, ionic, and polarizable compounds, including organic and inorganic ionic species (cations and anions), acids, amines, and ammonium salts. In addition to the classical determination of inorganic anions and cations in water and other aqueous solutions, IC-MS methods are rapidly gaining acceptance in regulated environments for the determination of polar anionic and cationic pesticides.

Unlike conventional liquid chromatography (LC), an ion chromatograph has a metal-free flow path with extremely low residual ionic chemical background. Unlike reversed-phase LC (RPLC) and hydrophilic interaction liquid chromatography (HILIC) columns, IC columns are typically hydrophilic, and rely on the ionic forces (ion-ion intermolecular interactions) to separate analytes. Although IC requires dedicated IC hardware, IC-MS/MS and LC-MS/MS methods can share a common mass spectrometer to boost return on investment and save laboratory bench space.

Anionic	Cationic
Glyphosate	Diquat
Glufosinate	Paraquat
Fosetyl-Al Bialaphos	Chlormequat
Phosphonic acid	Mepiquat
MPPA	N,N-Dimethylhydrazine
HEPA	Melamine
AMPA	Morpholine
N-acetyl AMPA	Trimethylsulfonium
N-acetyl glufosinate	Nereistoxin
Ethephon	Streptomycin
Cyanuric acid	Propamocarb
N-acetyl glyphosate	Cyromazine
Chlorate	Difenzoquat
Perchlorate	Matrine
	Oxymatrine



Achieve fast, reliable, and sensitive anionic polar pesticide quantitation

Anionic polar pesticide analysis challenges

Anionic polar pesticides include many frequently used worldwide, including glyphosate, glufosinate, and fosetyl-aluminum. Due to the complexity of food samples and high polarity of anionic pesticides, their simultaneous and sensitive analysis is challenging. Many polar anionic pesticides, including glyphosate, are zwitterions and exist in solution either as positively charged cations, negatively charged anions, or (at the isoelectric point) as overall neutral species, depending on pH. This characteristic makes their chromatographic separation by classic

HPLC techniques difficult. Traditionally, polar anionic pesticides have been determined individually using derivatization or ion pairing agents to overcome unwanted interactions during extraction and chromatographic separation.

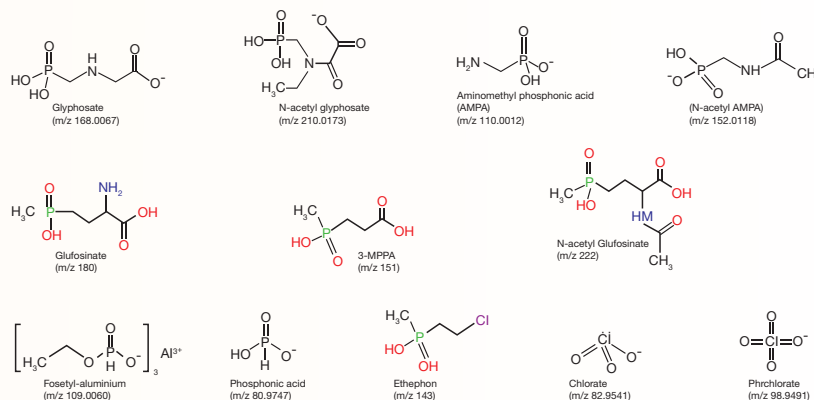
Multianalyte dilute-and-shoot method improves productivity, accuracy, and reproducibility

The Thermo Scientific™ IC-MS/MS workflow, which uses QuPPe™ extraction, is a sensitive, fast, and robust analytical solution for polar anionic pesticides analysis. The workflow enables routine identification and quantitation of multiple polar anionic pesticides in a simple clean-up then dilute-and-shoot method,

significantly enhancing productivity, accuracy and reproducibility.

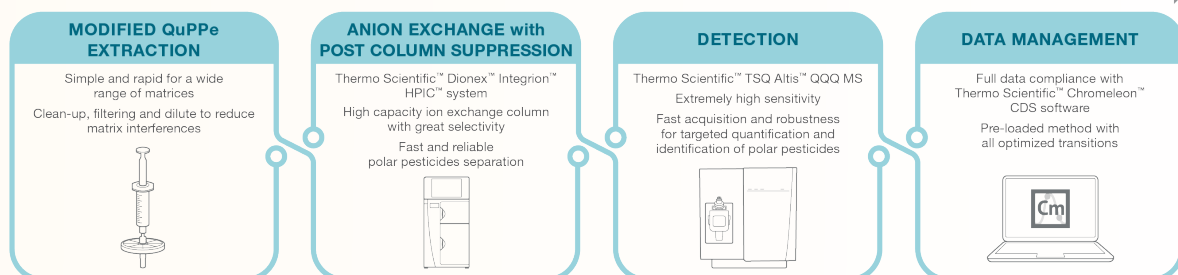
The IC-MS/MS workflow offers a considerable advance in ionic polar pesticide analysis. Though anionic polar pesticide residues often occur in foods, they are not always included in monitoring programs simply because they are not amenable to QuEChERS extraction and reversed phase LC-chromatographic separation.

To enhance sensitivity, Thermo Scientific™ Dionex™ high-capacity ion-exchange columns withstand higher sample loading, allowing analysis of low concentration polar analytes in difficult matrices such as cereal products.



Selected anionic polar pesticides ideally analyzed by IC-MS/MS.

ANIONIC PESTICIDES EXPLORER



Anionic polar pesticides analysis IC-MS/MS workflow

Anionic polar pesticides analysis workflow

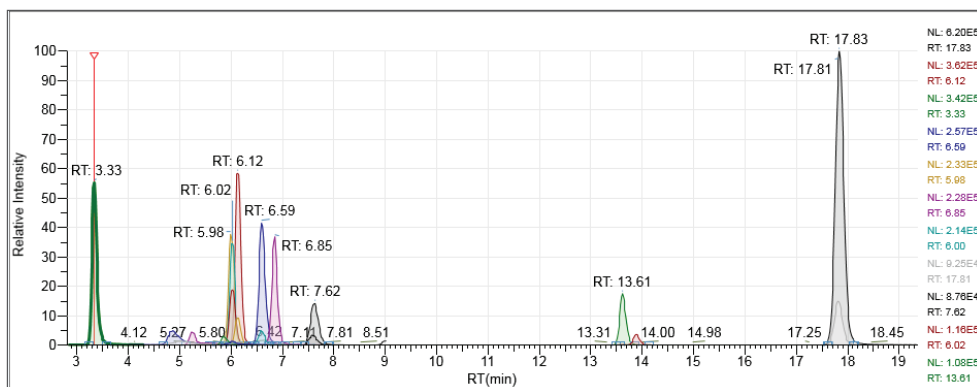
The anionic polar pesticides quantitation workflow begins with a modified QuPPE extraction with SPE cleanup to reduce matrix effects. Developed by the European Union Reference Laboratories for Single Residue methods (EURL-SRM), the QuPPE Method is the simple, rapid, and recommended approach to extract polar analytes from food samples. Analyte separation is efficient via a Dionex high-capacity anion exchange column on

either the Thermo Scientific™ Dionex™ Integriion™ HPIC™ or the Dionex ICS-6000 HPIC system equipped with conductivity detection. Post-column suppression reduces eluent background conductivity to enhance analyte conductivity. Suppression also minimizes accumulation of salts in the mass spectrometer interface and ion suppression in the source. High-sensitivity MS/MS detection relies on the Thermo Scientific™ TSQ Altis™ Plus triple quadrupole mass spectrometer. Data can be processed, analyzed, and

reported using either Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) or Thermo Scientific™ TraceFinder™ software.

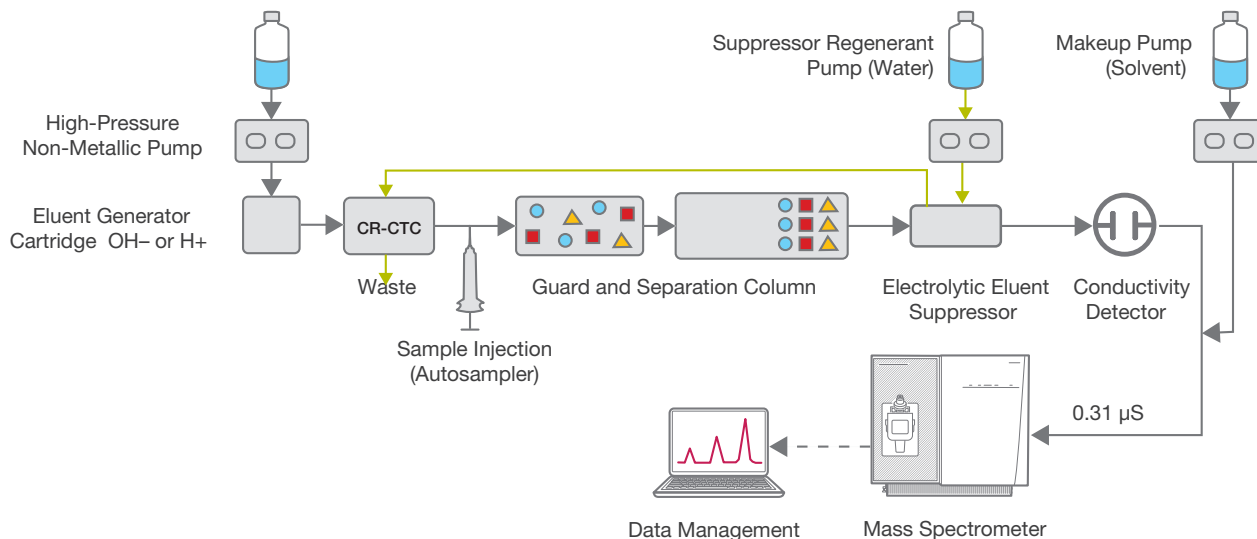
Sample-to-results solution

For an integrated sample-to-results solution the Thermo Scientific™ Anionic Pesticides Explorer provides a robust, validated off-the-shelf package built around the Dionex Integriion HPIC system and the Thermo Scientific™ Dionex™ IonPac™ AS19-4µm column set.



Analytes	RT / min
Fosetyl-AI	3.33
Bialaphos	5.25
Glufosinate	5.85
AMPA	5.97
HEPA	5.98
N-acetyl- AMPA	6.00
N-Acetyl-Glufosinate	6.02
Chlorate	6.12
MPPA	6.59
Phosphonic acid	6.85
Ethephon	7.62
Cyanuric acid	13.31
N-Acetyl-Glyphosate	13.61
Glyphosate	13.87
Perchlorate	17.83

Separation of anionic polar pesticides and metabolites by IC-MS/MS: glyphosate (N-acetyl glyphosate, AMPA, N-acetyl AMPA), glufosinate, (N-acetyl glufosinate, MPPA), ethephon (HEPA), fosetyl-aluminium (phosphonic acid), bialophos, cyanuric acid, chlorate, and perchlorate. Analyte retention times are highlighted at left. Separation of target anionic polar pesticides was performed in 21 minutes.

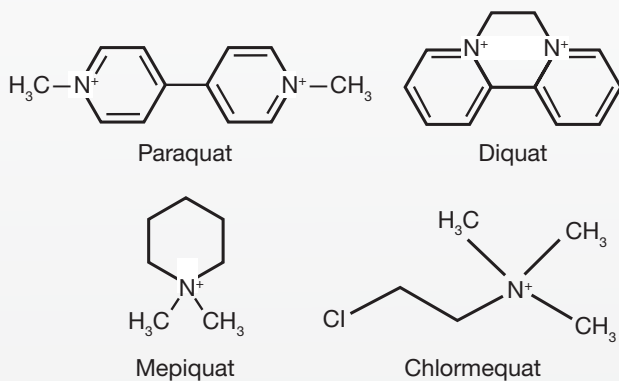


IC-MS/MS setup for the analysis of anionic polar pesticides.

Quantify difficult cationic polar pesticides using one IC-MS/MS system

Cationic polar pesticides add analytical challenges

Cationic polar pesticide determination in foods creates additional challenges due to their permanent charge nature. Some, for example diquat and paraquat, are doubly charged. Unlike anionic polar pesticides, the quaternary ammonium (Quats) subclass of cationic polar pesticides cannot exist as neutral species in solution at any pH. These unique structural and chemical features cause the Quats to tend to adhere (often non-reversibly) to many materials, particularly glass and metal, posing a significant challenge to quantitation. In addition, the critical pair diquat and paraquat differ only very slightly in molecular weight and hence require MS/MS for accurate quantitation.



Example quaternary ammonium (Quats) cationic polar pesticides

From modified QuPPE extraction with SPE cleanup and IC-MS/MS analysis to data processing, analysis and reporting, the cationic polar pesticide quantification workflow is essentially the same as that used for anionic polar pesticides. The only difference is that the IC setup uses the Thermo Scientific™ Dionex™ CR-CTC III

One IC-MS/MS system, two ionic polar pesticide workflows

By simply changing the eluent, column set, suppressor and the trap column, a Thermo Scientific IC-MS/MS system configured for anionic polar pesticides methods can also be used to analyze cationic polar pesticides. Plastic vials and all-PEEK components provide the metal-free and glass-free flow path needed to reliably deliver sticky cationic analytes to the triple quadrupole mass spectrometer.

Specifically designed to separate quaternary amine cationic polar pesticides, the Dionex IonPac CS21-Fast-4 μ m column is a high-capacity, hydrophilic cation exchange column that provides excellent peak shape and selectivity. The column features a large

separation window between monovalent and divalent cations, making it ideal for eluting most quaternary amine cationic polar pesticides between the alkali and alkaline earth metals. This large separation window is advantageous for samples that pose quantitation challenges, for example where amines are present at much lower concentrations than matrix cations.

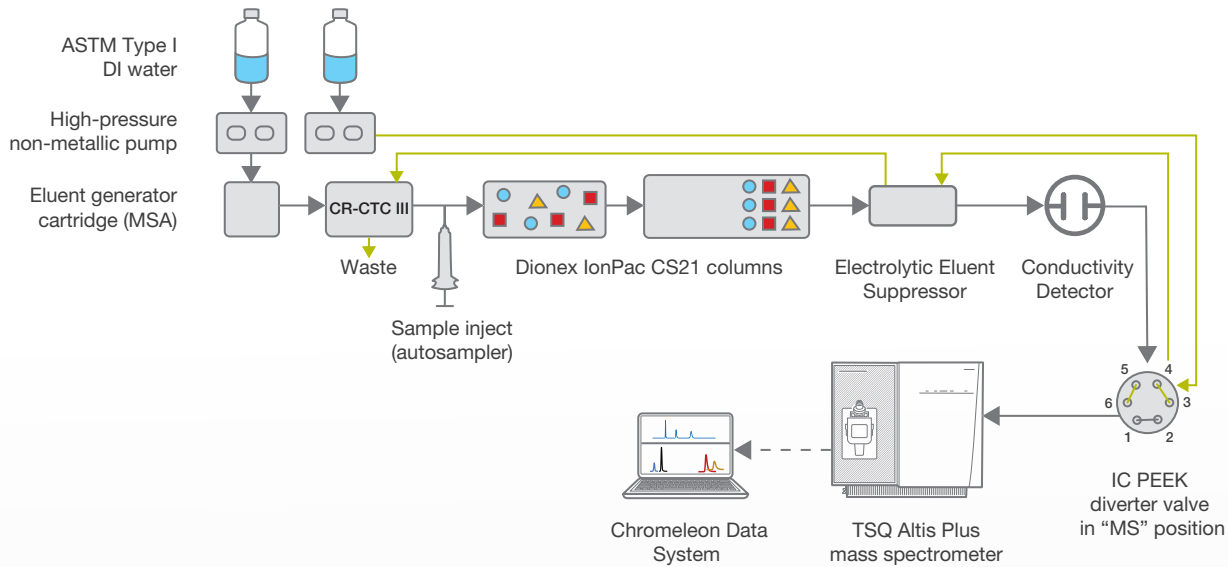


Dionex IonPac CS21-Fast-4m ion exchange column.

Continuously Regenerated Cation Trap Column, the Dionex IonPac CS21-Fast-4 μ m column, and Thermo Scientific™ Dionex™ CDRS 600 suppressor instead of the Thermo Scientific Dionex CR-ATC 600 continuously regenerated trap column, Dionex high-capacity anion exchange column, and the Dionex ADRS 600

suppressor. Therefore, all the advantages of the IC-MS/MS anionic polar pesticides workflow—simplified, time-saving sample preparation, and enhanced accuracy and reproducibility—can be achieved for cationic polar pesticides analysis.

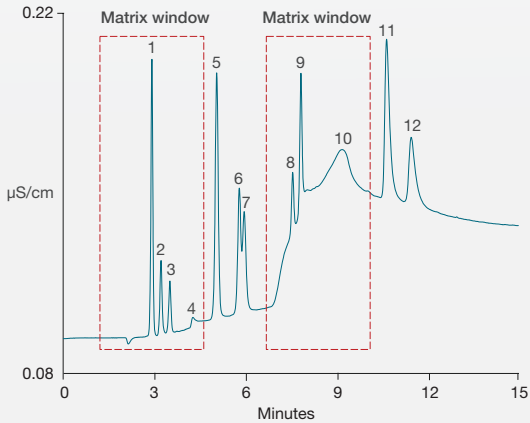
Cationic polar pesticides analysis workflow



IC-MS/MS setup for the analysis of cationic polar pesticides.

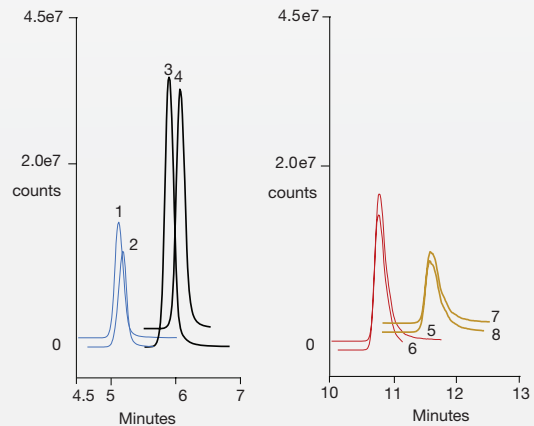
Columns: Dionex IonPac CS21-Fast-4 μ m and guard, 2 mm i.d.
 Eluent source: Dionex EGC 500 MSA, Dionex CR-CTC III trap column, HP EG degas kit
 Eluent: Methanesulfonic acid (MSA) gradient
 Gradient: 3 mM (-4 to 0 min), 3-6 mM (0 to 3.6 min), 6-22 mM (3.6 to 6 min), 22-25 mM (6 to 15 min), 3 mM (15 min)
 Flow rate: 0.30 mL/min
 Injection volume: 10 μ L
 Column temp.: 40 $^{\circ}$ C
 Detection 1: Suppressed conductivity, 20 $^{\circ}$ C, Dionex CDRS 600, 2 mm, 22 mA, external water mode
 Auxiliary pump: 0.3 mL/min for DI water regenerant

Peaks:	1.	2.	3.	4.	5.	6.	7.	8.	9.	10.	11.	12.
	Sodium	Ammonium	Potassium	Unknown	Chlormequat	Mepiquat-d ₄	Mepiquat	Magnesium	Calcium	System peak	Paraquat	Diquat
	30 μ g/L	10	10	--	50	50	50	10	20	--	50	50



Detection 2: TSQ Altis Plus triple quadrupole, +HESI-II, +2.8 kV, SRM mode
 Desolvation: None
 MS N₂ gases (arb): Sheath: 45; Aux: 3; Sweep: 2
 Source temp.: Vaporizer: 300 $^{\circ}$ C; Ion transfer tube: 350 $^{\circ}$ C
 SRM Polarity: Positive
 SRM Cycle time (s): 0.8 s
 SRM Resolution (FWHM): Q1: 0.7; Q3: 1.2
 SRM CID gas (mTorr): 1.5
 SRM Source frag. (V): 10
 SRM Chromatog.: Peak width: 6 s; Filter
 Standard: 5 μ g/L

Peaks:	Precursor (m/z)	Product (m/z)	Collision energy (V)
1.	126	57.9	30
2.	122.1	57.9	30
3.	130	110	30
4.	114.1	98.1	30
5.	97	179	19
6.	93	171	19
7.	96	88.5	19
8.	92	157.1	19



IC (left) and SRM (right) chromatograms showing separation of mixed cations and resolution of quaternary amine pesticide standards.

Advance quantitative workflows and increase productivity with a complete Thermo Scientific IC-MS/MS system

Whether it's just a few samples or a heavy workload, routine or challenging analyses, Thermo Scientific offers an innovative and robust IC system to meet your performance and affordability requirements for pesticides analysis.



Dionex Integrion HPIC System: Run routine methods

Achieve versatile and efficient separations that meet routine ion analysis demands with the reliable Dionex Integrion HPIC system. Its high-pressure ion chromatography (HPIC) capabilities enable faster analysis without compromising data quality. The Dionex Integrion HPIC system is available in a wide range of configurations.

Dionex ICS-6000 HPIC System: Run different methods simultaneously

The modular Dionex ICS-6000 HPIC system is a highly configurable system with capillary IC capabilities. It enables you to develop and run different methods for single sample or multiple samples simultaneously. Its robust design allows operation up to 5000 psi and produces consistent, reliable results for challenging pesticide analysis.

Automated eluent generation (EG): Improve reproducibility, save time and money

Eluent generation (EG) cartridges electrolytically produce high-purity hydroxide, carbonate, and methanesulfonic acid (MSA) eluents for isocratic and gradient runs in RFIC systems. There is no need to manually prepare eluent, only a high-purity source of deionized water is needed. Optional Reagent-Free Ion Chromatography with Eluent Generation (RFIC-EG) combines automated EG and electrolytically regenerated suppressors to create eluents (at the desired concentration).



Thermo Scientific™ Dionex eluent suppressors: Achieve low detection limits

Modern IC is performed with suppressed conductivity detection using a device called a suppressor. Suppressors remove conductive ions from the eluent, thereby increasing analyte signal while decreasing background signal and noise, enabling the highest sensitivity for the determination of inorganic analytes by conductivity detection. The device also prevents mass spectrometer corrosion, salt accumulation in the entrance aperture and skimmer, and ion suppression in the source.

Choice of common software platforms for pesticides analysis by chromatography and MS

When you choose Thermo Fisher Scientific GC, LC, and IC-MS systems for pesticide analyses, laboratory staff only need to learn and operate one software platform. This helps laboratories streamline and standardize operating procedures, minimize training requirements, and simplify lab operations. Both Chromeleon CDS and TraceFinder software platforms can be used to control instruments, and acquire, process and report data.



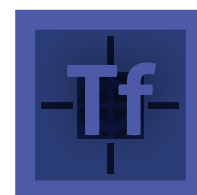
TSQ Altis Plus Triple Quadrupole Mass Spectrometer: Achieve ultimate quantitative performance

With superior acquisition speeds, enhanced sensitivity, excellent selectivity, and exceptional robustness. The TSQ Altis Plus mass spectrometer delivers unprecedented accuracy and precision trace-level pesticide detection and quantitation in complex matrices. The instrument control software is intuitive and the simplified calibration approach consolidates steps into an intelligent instrument check and calibration routine.



Chromeleon CDS: Your all-in-one software solution for targeted pesticide workflows

Drive productivity and lower training and maintenance efforts with the intuitive Chromeleon CDS. Providing all the tools needed to expedite data review, such as dual sequence processing capabilities, automatic flagging options and customized view settings. Enable your lab to deliver reliable results in a shorter time frame whilst enabling quantification and identification of pesticide residues in accordance to SANTE guidelines. Delivering comprehensive compliance and data integrity to your laboratory.



TraceFinder software: Simplify high-throughput screening and quantitation

Driven by a powerful and intuitive set of intelligent acquisition and data processing tools, TraceFinder software provides rapid access to results and increases output across the entire laboratory. Smart sample flagging, flexible data review, and custom report generation remove the bottlenecks associated with data review and simplify sample analysis at each step. TraceFinder software enables control of multi-channel LC, single quadrupole, triple quadrupole and high-resolution LC-MS systems, as well as IC and GC systems.

There's no time for downtime

Thermo Scientific supports your IC-MS system from installation and warranty to service plans and compliance services. Our full range of services helps ensure you get the best performance from your system throughout its life. We can put together services to best fit your needs, so your equipment operates reliably and efficiently.



Almanac web-based monitoring and management

Stay connected to your science. See how the Thermo Scientific™ Almanac™ application can help you get the most out of your instruments.

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Technical and online support: peak performance for your instruments

Helping you keep your instruments running at peak performance is our goal. Whether you're looking for an instrument manual or spare parts, want to submit a repair request, or check on the status of your warranty or service contract, we have every support option you're looking for.

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