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THE POWER OF MASS SPECTROMETRY FOR IC ANALYTICAL CHEMISTS



Unleash New Possibilities
with Enhanced Detection for IC Applications

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THE POWER OF MASS SPECTROMETRY

Ion chromatography (IC) excels in analyzing ionic species—analytes of major importance to environmental, food and beverage, pharmaceutical, life science, chemical, power generation, and electronics industries. As the ion chromatography innovator and technology leader for over 40 years, Thermo Fisher Scientific understands what IC analytical chemists need for their work.

There is a continuing need for today's researcher to detect small quantities of analytes in complex samples. But what if you need even lower levels of sensitivity and selectivity to add extra confidence to your results?

Unleash New Possibilities with Enhanced Detection for IC Applications

Combining ion chromatography (IC) with mass spectrometry (MS) maximizes the power to detect unexpected coelutions of components and confirm trace components with the analytical confidence of mass spectrometry. Mass spectrometry dramatically improves your IC system capabilities and provides:

- Higher sensitivity and accurate quantitation
- Peak confirmation and evaluation of chromatographic peak purity
- Improved resolution of complex samples
- Seamless integration of MS data into your IC workflow

Coupling IC to MS

IC-MS is a recommended method for sensitive and selective determinations of ions. Combining ion chromatography with MS workflows increases efficiency and sensitivity, and improves resolution in complex samples, leading to more accurate quantitation, improved confidence, and more chemical information about every sample.

Thermo Fisher Scientific offers several different mass spectrometer options for IC systems:

- single quadrupole MS
- triple quadrupole MS
- high resolution-accurate mass (HRAM) hybrid quadrupole-Orbitrap MS

As the capabilities of these instruments grow, so does their power to provide information about your compounds of interest. While a single quadrupole MS adds sensitivity and peak confirmation to your analyses, a triple quadrupole MS/MS provides additional sensitivity, peak confirmation, and basic structural elucidation. HRAM Orbitrap MS adds advanced structural elucidation to IC-MS analyses.

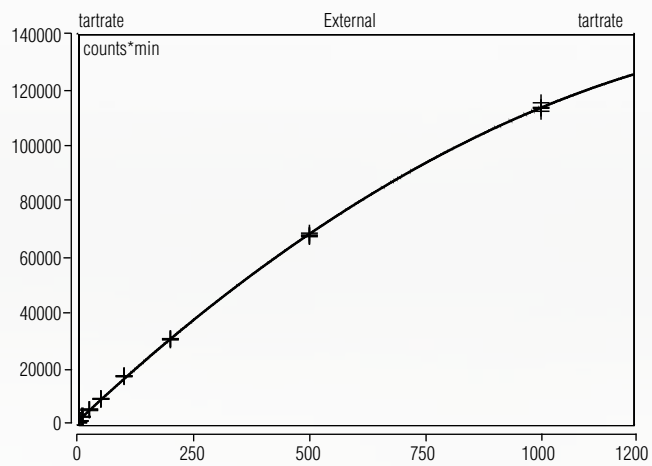


MORE CONFIDENCE

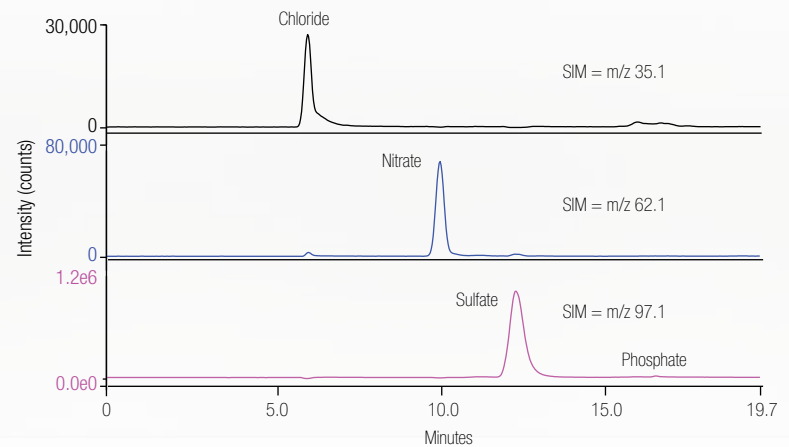
Higher Sensitivity and Accurate Quantitation

For routine analyses where single digit parts-per-billion (ppb) sensitivities are required, a simple mass detector, such as a single quadrupole mass spectrometer, offers the required sensitivity. Mass detection adds confidence to your quantitation, enabling you to obtain limits of detection (LODs) at least an order of magnitude greater than those provided by conductivity detection.

With the use of very specific MS selected ion monitoring (SIM) detection, ppb-level quantification can be performed with greater confidence on a wide range of real-world samples, such as bottled drinking water.



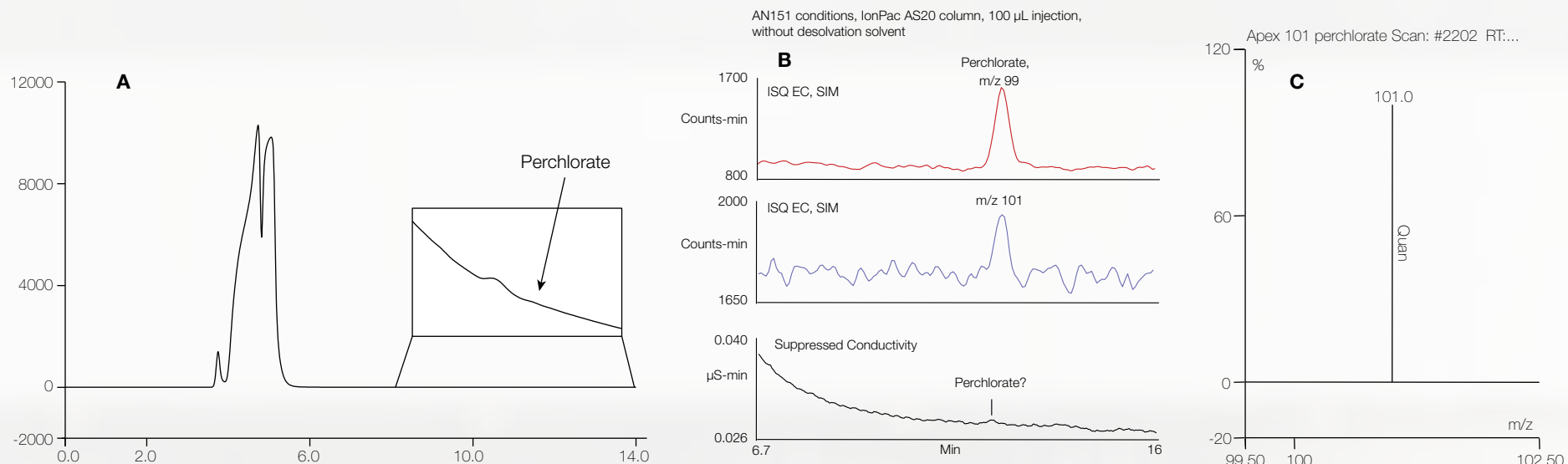
Calibration curve of tartrate at concentrations from 2 ppb to 1000 ppb, $r^2=0.9998$



Anions in a bottled water sample

Peak Confirmation

In addition to the enhanced detection, if your study requires peak confirmation or peak purity analysis the single quadrupole MS detector such as the Thermo Scientific™ ISQ™ EC mass spectrometer will provide complementary molecular weight data, for an increased degree of confidence.



Determination of perchlorate in a Municipal Drinking Water Sample. (A) The conductivity channel provides very limited sensitivity towards the perchlorate peak and no confirmatory data. (B) SIM m/z 99 provides a very sensitive response towards perchlorate. (C) SIM m/z 101 confirms the response as perchlorate by confirming the 3:1 ratio of m/z 99:101 expected for perchlorate.

Where unknown chromatographic peaks appear, mass detection enables the IC analytical chemist to quickly and effectively suggest a number of possibilities for these unknown peaks. By scanning across a chromatographic peak with a mass detector, it is possible to detect the appearance of unusual masses.

FLEXIBLE IC-MS COMBINATIONS

Thermo Fisher Scientific offers two different IC systems, the Thermo Scientific™ Dionex™ ICS-6000 HPIC™ system and the Thermo Scientific™ Dionex™ Integriion™ HPIC™ system, suited for pairing with MS detection. Each of these unique IC systems can be used with a variety of mass spectrometers, offering increasing levels of confidence, peak confirmation, and structural elucidation for your analyses.

Dionex ICS-6000 HPIC system:

A modular, highly flexible IC system designed to meet the widest range of applications.

Dionex Integriion HPIC system

A compact, integrated IC system for routine ion analysis demands, ease-of-use and reliability.

Thermo Scientific™ ISQ™ EC

Single Quadrupole Mass Spectrometer: An economical, benchtop mass detector designed for routine IC-MS workflows.



<i>Mass Spectrometer</i>	<i>Analyzer</i>	<i>Mode of Operation</i>	<i>MS</i>	<i>MS/MS</i>	<i>Sensitivity</i>	<i>Peak Confirmation</i>	<i>Structural Elucidation</i>
ISQ EC	Quadrupole	Single ion monitoring (SIM)	●	◐	◐	◐	◐
TSQ Quantis MS	Triple Quadrupole	Selected reaction monitoring (SRM)	●	●	◐	◐	◐
TSQ Altis MS	Triple Quadrupole	Selected reaction monitoring (SRM)	●	●	●	◐	◐
Q Exactive MS	Orbitrap mass analyzer	High Resolution Accurate Mass (HRAM)	●	●	◐	●	◐
Orbitrap Fusion MS	Orbitrap mass analyzer	High Resolution Accurate Mass (HRAM)	●	●	◐	●	●

Thermo Scientific™ TSQ Altis™ and Thermo Scientific™ TSQ Quantis™ Triple Quadrupole Mass Spectrometers: Best-in-class benchtop MS designed for quantitative performance, robustness, and value.

Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap Mass Spectrometer: High-resolution, accurate-mass (HRAM) benchtop MS that delivers high resolution data for quantitative, screening and confirmation studies.

Thermo Scientific™ Orbitrap Fusion™ Mass Spectrometer: An instrument combining the best of quadrupole, ion trap and Orbitrap mass analysis and ease of use for the highest performing research system particularly suited for life science applications.

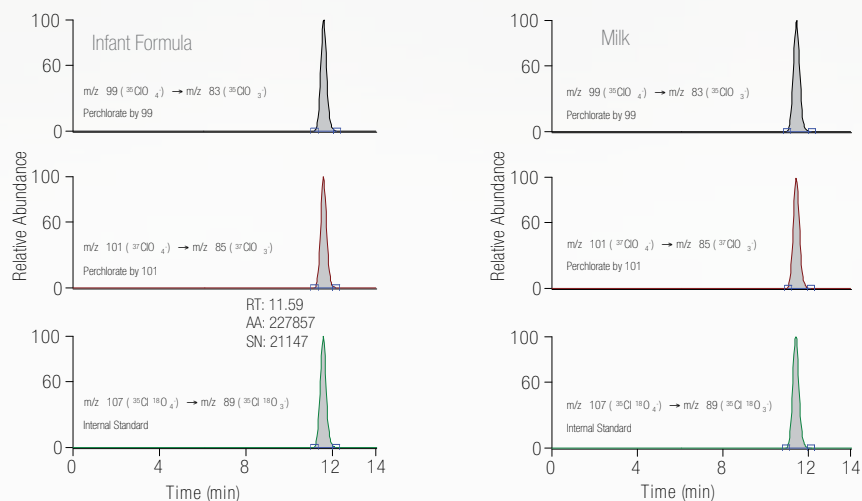


RESOLVING COMPLEXITY



Increased Selectivity for Complex Samples

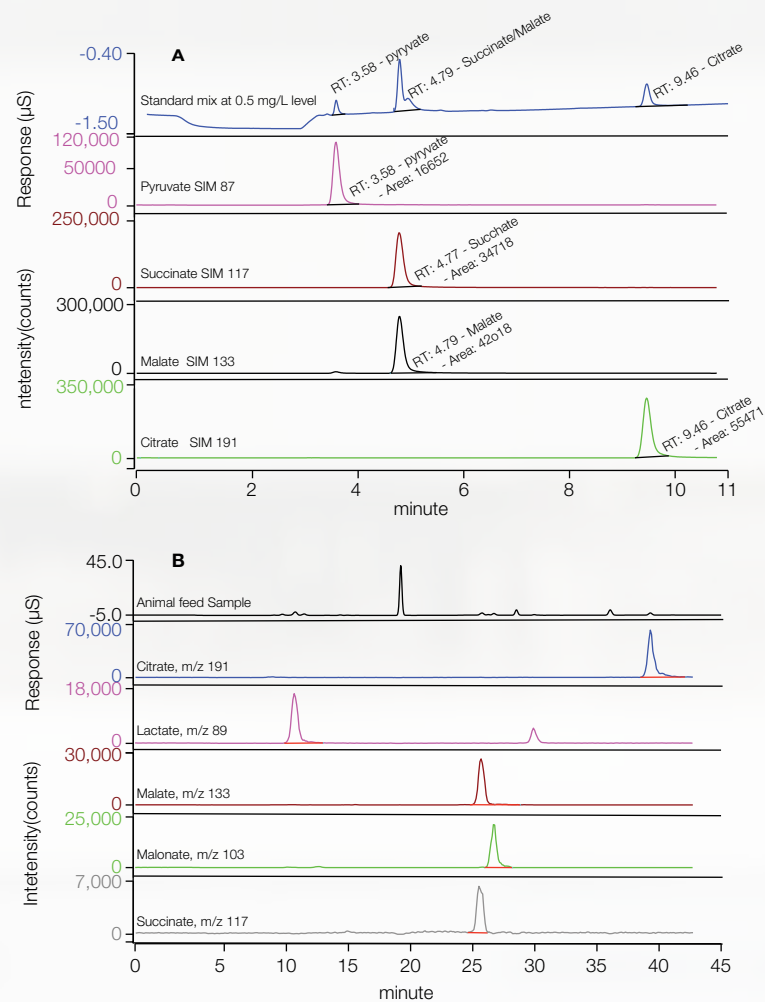
When you need increased sensitivity and peak confirmation, the increased power of a triple quadrupole MS may be the answer. The sensitivity and selectivity of MS/MS detection makes it a highly preferred method for complex sample matrices. For example, perchlorate in baby formula can be quantified, without enrichment at low parts-per-trillion (ppt) levels using simple sample preparation and a TSQ Altis triple quadrupole mass spectrometer for detection. This system provides excellent reproducibility, accuracy, and precision.



Perchlorate in unspiked infant formula and milk samples. Calculated concentrations are in the 1–5 $\mu\text{g/L}$ range.

Selectivity for Co-Eluting Peaks

Combining ion chromatography with mass spectrometric detection offers great selectivity. In the example to the right, organic acids were analyzed by IC-MS. Using MS detection, each of these organic acids was observed as a single peak. By overlaying the individual responses for each recorded mass, it is possible to determine how the co-eluting organic acids contribute to the total chromatographic peak.

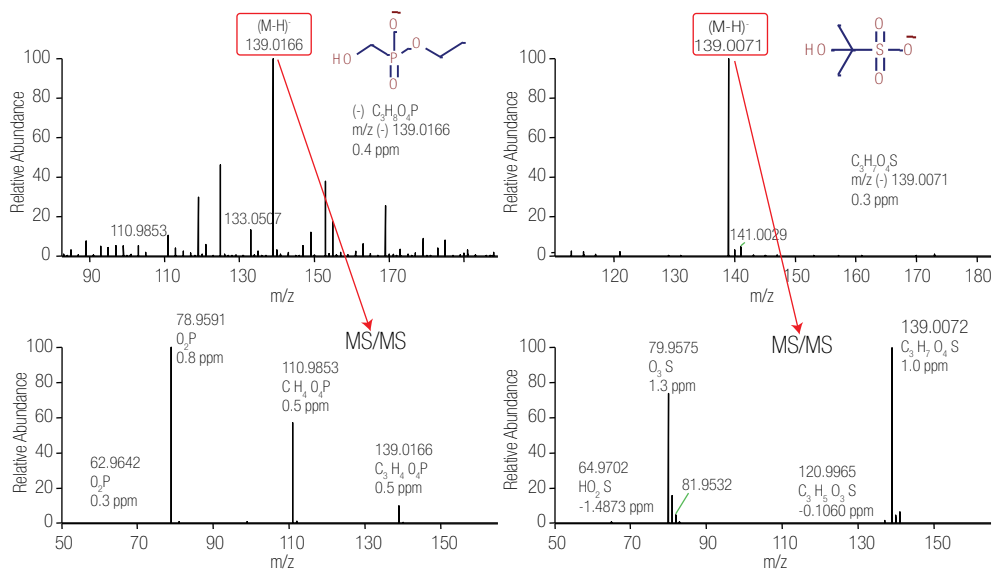


Determination of organic acids in Animal Feed by single quadrupole IC-MS. (A) The conductivity channel provides sufficient response for the organic acids, but lacks resolution for malate, malonate and succinate. (B) The highly selective SIM channels on the Thermo Scientific ISQ EC are able to respond individually to the three co-eluting organic acids, providing both quantitative and qualitative data.

Structural Elucidation Capabilities

IC combined with high-resolution, accurate-mass (HRAM) Orbitrap mass spectrometry is an ideal solution for component identification in non-targeted and unknown workflows. For example, identification of lithium-ion battery failure analysis products using HRAM MS/MS offers four-decimal-point accuracy to distinguish between species.

The unique fragmentation signature enhances that confidence. In addition to validating a proposed degradation pathway, confidence in the results avoids spending research time and resources going in an unproductive direction.



HRAM MS/MS fragments facilitate identification of unknown compounds.

IC-MS Analysis Software

Thermo Scientific offers a range of software solutions to support IC-MS applications.

- Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software is ideal for routine quantitative workflows.
- Thermo Scientific™ TraceFinder™ and/or Thermo Scientific™ Xcalibur™ software is recommended for qualitative workflows.

Find out more at thermofisher.com/ICMS

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