

## Haloacetic acids (HAAs) in drinking water

Determination of disinfection by-products  
by validated IC-MS/MS application workflow

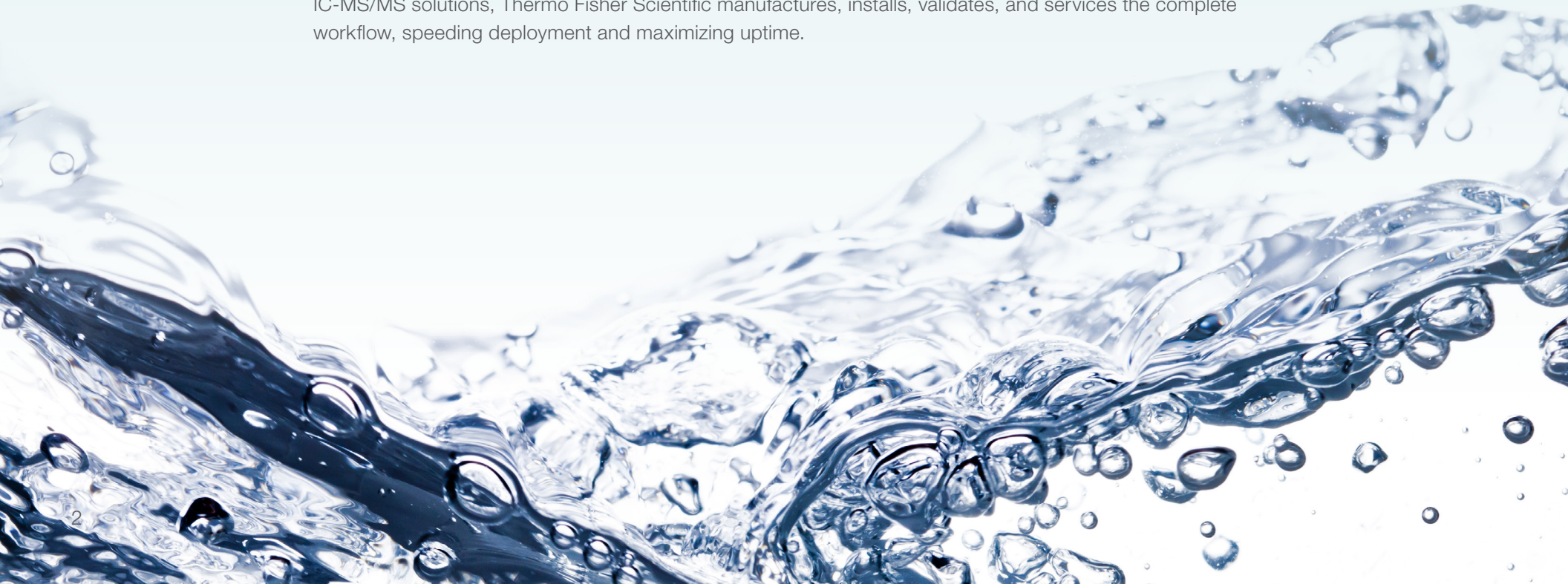
# Ensure safe drinking water—rapidly and cost-effectively

## Accelerate your haloacetic acids, bromate, and dalapon analyses

Disinfection is important in ensuring the supply of pathogen-free drinking water. However, excessive consumption of disinfection by-products (DBPs) like haloacetic acids (HAAs), bromate, and dalapon can result in health issues. With increasing regulatory focus on DBPs, drinking water facilities around the world need hands-off, high-throughput analyses of these contaminants.

That's the reason for the Thermo Scientific™ Disinfection By-Products Application Workflow. Comprised of an integrated Thermo Scientific ion chromatography-tandem mass spectrometry (IC-MS/MS) system with direct injection to eliminate sample preparation, this workflow provides rapid, cost-effective drinking water testing per United States Environmental Protection Agency (U.S. EPA) Method 557.

Compared to gas chromatography-electron capture detection (GC-ECD) per U.S. EPA Method 552.3, this workflow does away with time-consuming and complicated manual sample preparation steps. Unlike other IC-MS/MS solutions, Thermo Fisher Scientific manufactures, installs, validates, and services the complete workflow, speeding deployment and maximizing uptime.





### Meet global requirements

From the United States Safe Drinking Water Act (SDWA), to the European Commission (EC) Right2Water initiatives and emerging regulations in China, government regulations and proposals are driving needs for more efficient DBPs monitoring. The Thermo Scientific DBPs Application Workflow is ideally suited to meet the requirements described by the U.S. EPA and the EC.



### Increase sample throughput, reduce costs

There are two U.S. EPA methods for HAAs analysis: GC-ECD Method 552.3 and the more recent IC-MS/MS Method 557. Besides differences in the instrument technology used, the methods differ in sample preparation requirements. Time consuming and labor intensive, U.S. EPA Method 552.3 requires multiple extraction steps and derivatization exceeding four hours. U.S. EPA Method 557 uses direct injection without sample preparation, offering significantly higher sample throughput. For labs running more than 24 batches of 25 samples per month, the DBPs Application Workflow can provide substantial operational cost savings.



### Broaden analytical scope

U.S. EPA Method 557 can be used to directly determine bromate and dalapon in drinking water samples, broadening analytical scope. One IC-MS/MS system can analyze anionic polar pesticides such as glyphosphate and glufosinate, as well as anionic environmental compounds such as bromide and perchlorate.



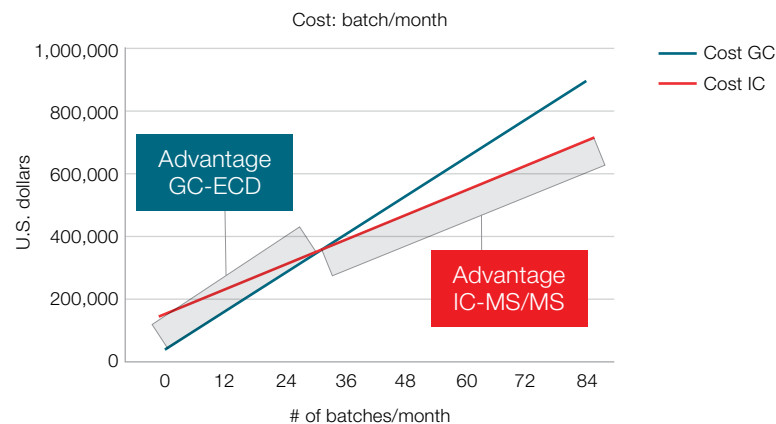
### Achieve reliable results, meet proficiency standards

Ion chromatography (IC) offers significant benefits for the determination of HAAs due to its ability to efficiently separate polar molecules. Mass spectrometry (MS) detection provides the sensitivity and selectivity required to obtain reliable analytical results using direct injection. Compared to GC-ECD, IC-MS/MS provides better recoveries, making it easier to meet proficiency standards.

Analyte	Minimum reporting level (MRL) goal U.S. EPA/EC	Maximum contaminant level (MCL) goal U.S. EPA/EC	HAA5 compounds*	HAA9 compounds
Dichloroacetic acid (DCAA)	0.2 µg/L	0 µg/L	✓	✓
Monochloroacetic acid (MCAA)	2.0 µg/L	70 µg/L	✓	✓
Trichloroacetic acid (TCAA)	0.5 µg/L	20 µg/L	✓	✓
Monobromoacetic acid (MBAA)	0.3 µg/L	—	✓	✓
Dibromoacetic acid (DBAA)	0.3 µg/L	—	✓	✓
Bromochloroacetic acid (BCAA)	0.3 µg/L	—	—	✓
Bromodichloroacetic acid (BDCAA)	0.5 µg/L	—	—	✓
Chlorobromoacetic acid (CDBAA)	0.3 µg/L	—	—	✓
Tribromoacetic acid (TBAA)	2.0 µg/L	—	—	✓
Bromate	10 µg/L	—	—	—
Dalapon	200 µg/L	—	—	—

\* The U.S. EPA and EC MCL for sum of the HAA5 compounds is 60 µg/L.

The DBPs Application Workflow is ideally suited to meet the method requirements specified by the U.S. EPA/EC.

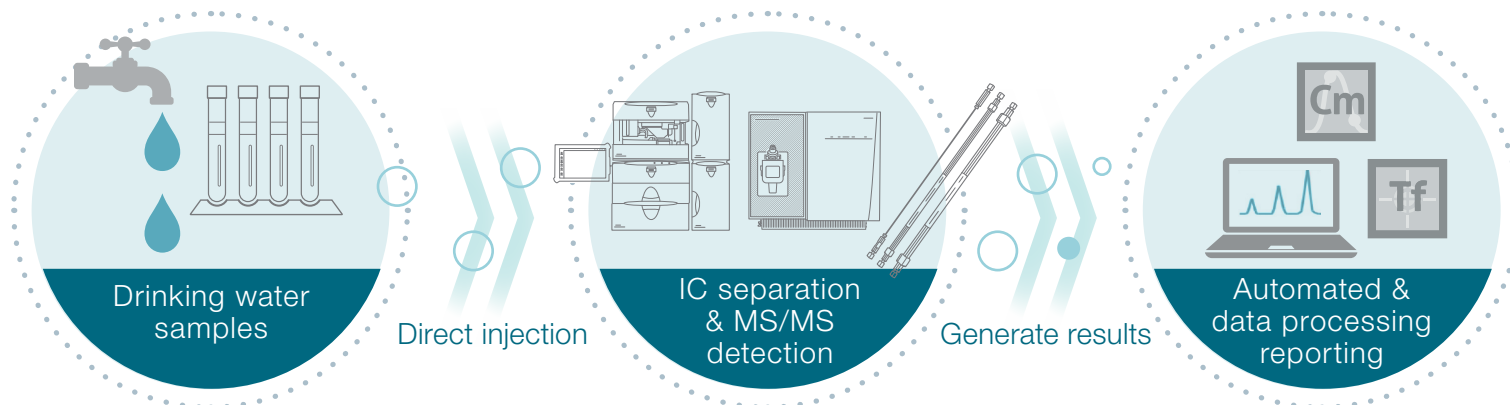


Cost of ownership comparison. Relative cost savings and throughput advantages of GC-ECD and IC-MS/MS are based on instrument price, sample cost, labor cost, and sample prep time. A linear graph mapping the cost savings and sample throughput, using an online cost of ownership calculator, provides a visual means of deciding on an instrument system based on the slope and the intersection of the two lines with respect to cost (y-axis) and batch volume (x-axis).

# Access a proven workflow, state-of-the-art technology

The DBPs Application Workflow provides proven reliability based on integrated high-performance IC-MS/MS components sold and supported by a single trusted manufacturer. Thermo Fisher Scientific is the only vendor today that provides a complete validated system for DBPs testing per U.S. EPA Method 557. Unlike other systems, the workflow includes proven methods that provide confidence and time savings. To get you up running samples quickly and minimize downtime, the complete system is validated at our factory, and at time of installation and servicing.

Water samples can be directly injected into the IC system for separation and subsequent MS/MS detection. Automated data processing and reporting are used to generate results.



## Significant increases in resolution and throughput

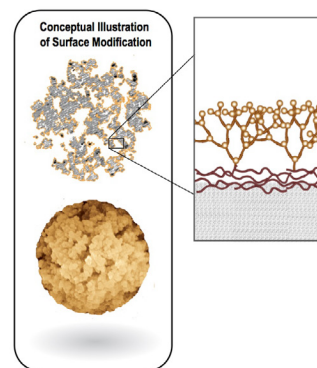
### Dionex ICS-6000 Standard Bore and Microbore HPIC systems

The Thermo Scientific™ Dionex™ ICS-6000 HPIC™ System is reliable, economic, and environmentally friendly for the separation of HAAs, bromate, and dalapon. Get significant increases in resolution and throughput, address a full range of IC applications, and solve complex analytical challenges with duality, modularity, capillary/hybrid operation, and ultimate versatility. The system can operate continuously when configured as a Thermo Scientific™ Reagent-Free™ IC (RFIC™) System to automate creation of IC eluents and regenerants, reduce labor and solvent costs, and achieve highly reproducible separations.

## Excellent separation

### Dionex IonPac AS31 analytical and guard columns

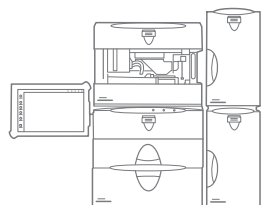
The selectivity of the Thermo Scientific™ Dionex™ IonPac™ AS31 Column provides excellent separation of the nine HAAs, bromate, and dalapon in drinking water from common anions such as chloride, sulfate, and carbonate. For fast analysis, the column provides 39% shorter run times relative to the Thermo Scientific™ Dionex™ IonPac™ AS24 Column, reducing U.S. EPA Method 557 run time from 57 to 35 min. The column has a high capacity to allow large loop injections for trace analysis ( $\mu\text{g/L}$ ) without sample preconcentration.



The Dionex IonPac AS31 column stationary phase consists of a novel, hyper-branched anion-exchange condensation polymer, electrostatically attached to the surface of a sulfonated wide-pore polymeric substrate. With the Dionex ICS-6000 HPIC system and the column held to 15°C, sample integrity is ensured.

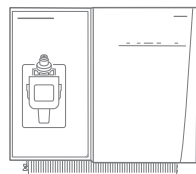
## Confident quantitation

For highest confidence in quantitation choose the Dionex ICS-6000 HPIC system and the Thermo Scientific™ TSQ Fortis™ Triple Quadrupole Mass Spectrometer. The sensitivity provided by these instruments make it possible to perform direct injection of drinking water samples, eliminating complex and variable sample preparation.



### Dionex ICS-6000 HPIC system

Suppressors remove conductive ions from the eluent, thereby increasing analyte signal while simultaneously decreasing background signal and noise. Our reagent-free IC (RFIC) systems with eluent generation (RFIC-EG) combine automated eluent generators and electrolytically regenerated suppressors to electrolytically create the required eluents and regenerants used for IC applications. Plumb in a clean source of deionized water, and the RFIC-EG system takes care of the rest.



### TSQ Fortis mass spectrometer

Achieve new levels of confidence and maximum productivity. The instrument offers intuitive, workflow-driven software solutions that support various applications. Its robust design ensures reliable and consistent results for users of all skill levels.

## Productivity driven

Powerful, productive data acquisition processing, and management is by Thermo Scientific™ TraceFinder™ Software and Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) Software.



### TraceFinder software

Simplify high-throughput screening and quantitation. Driven by a powerful and intuitive set of data acquisition and processing tools, the software provides rapid access to results and increases output across the lab. TraceFinder is the software platform familiar to existing MS users and is best suitable for routine, production, and high-throughput laboratories.



### Chromeleon CDS software

Streamline your workflows. Built with the lab and IT in mind, the software delivers superior compliance tools, networking capabilities, instrument control, automation, data processing, and more. It's an enterprise solution designed for tracking, accountability, and QA/QC that is incredibly easy to use, with fewer mouse clicks, and more "right-first-time" results. It's also designed to scale globally and provide strong return on investment.



## Disinfection by-product formation and pesticide contaminants

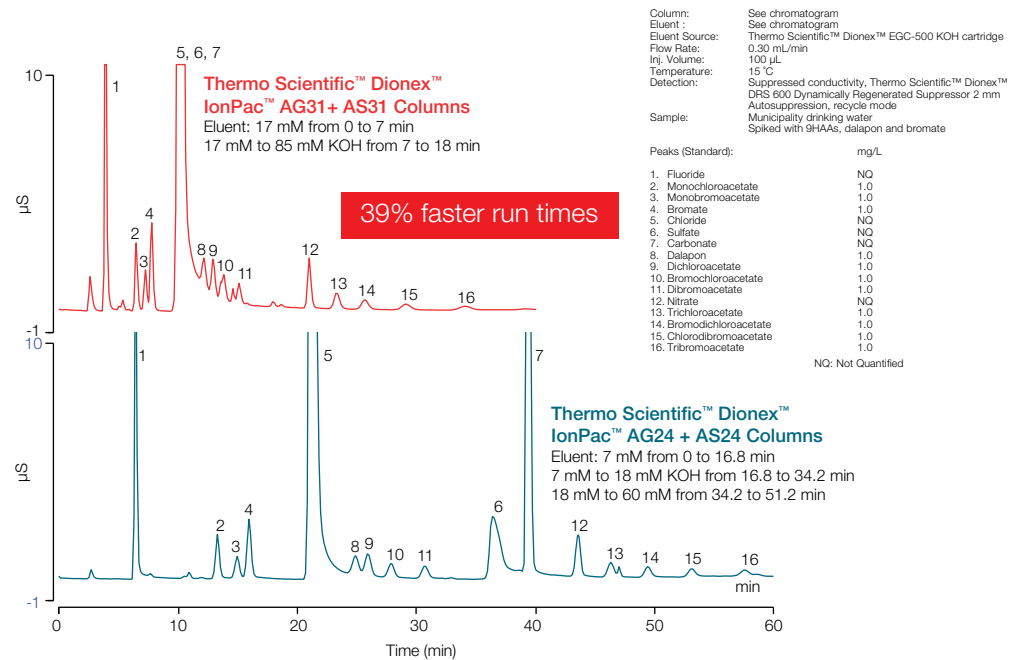
- Nine major HAAs are formed during chlorination of drinking water containing natural organic matter and bromide
- Used to address chlorine resistant organisms, ozonation of drinking water containing bromide can result in the formation of bromate, a potential carcinogen even at low µg/L concentrations
- Dalapon is an herbicide used to control grasses in a wide variety of crop and non-crop applications and can move in water courses by soil erosion. It is associated with minor kidney changes.

# Directly inject samples, perform faster separations, achieve higher throughput and repeatability

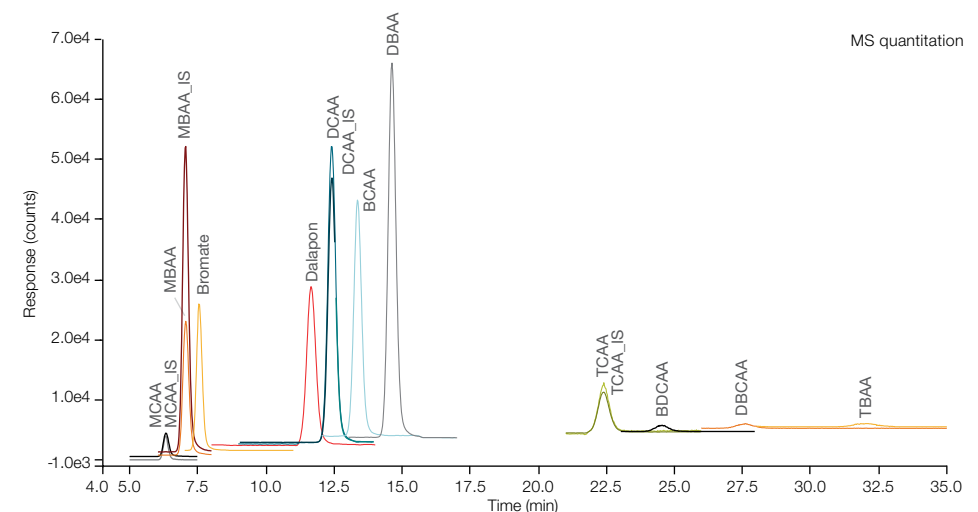
Laboratories approaching the limits of their GC-ECD systems can substantially benefit from adopting the DBPs Application Workflow by IC-MS/MS. The workflow enables easy implementation of a rapid, reliable, and reproducible solution for quantitation of nine HAAs, bromate, and dalapon in water per U.S. EPA Method 557 using IC-MS/MS. This workflow leverages the robust sensitivity performance of both the Dionex ICS-6000 system and the TSQ Fortis mass spectrometer to address the analytical challenges of drinking water analysis while reducing time and cost per sample.

## The DBPs Application Workflow is preferred when there are:

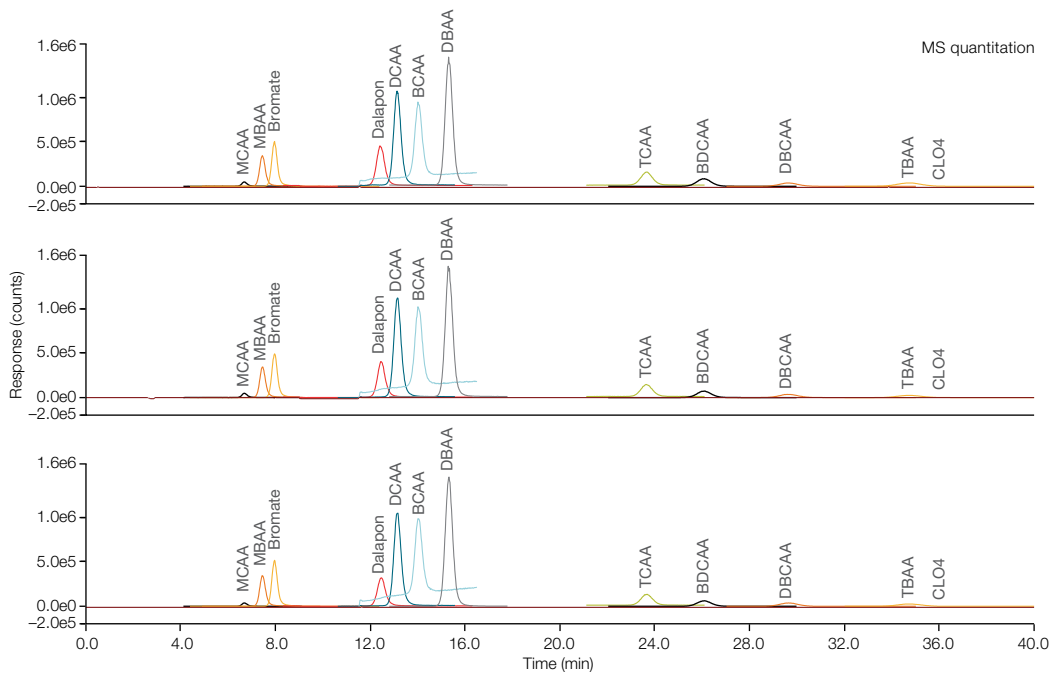
- Limited time and personnel to perform all analyses required of the laboratory and thus a need to reduce labor intensive tasks, such as liquid-liquid solvent extractions and derivatization
- Needs for a reliable technique to reduce repeat analyses
- Multiple inorganic analytes that need testing
- Faster sample-to-results turn over times are needed
- Concerns about the use of organic solvents and the associated costs of the chemical waste disposal



Separation of HAAs, bromate, and dalapon in drinking water using the Dionex IonPac AS31 (top trace) and Dionex IonPac AS24 (bottom trace) columns. The Dionex IonPac AS31 column provided 39% faster run times.

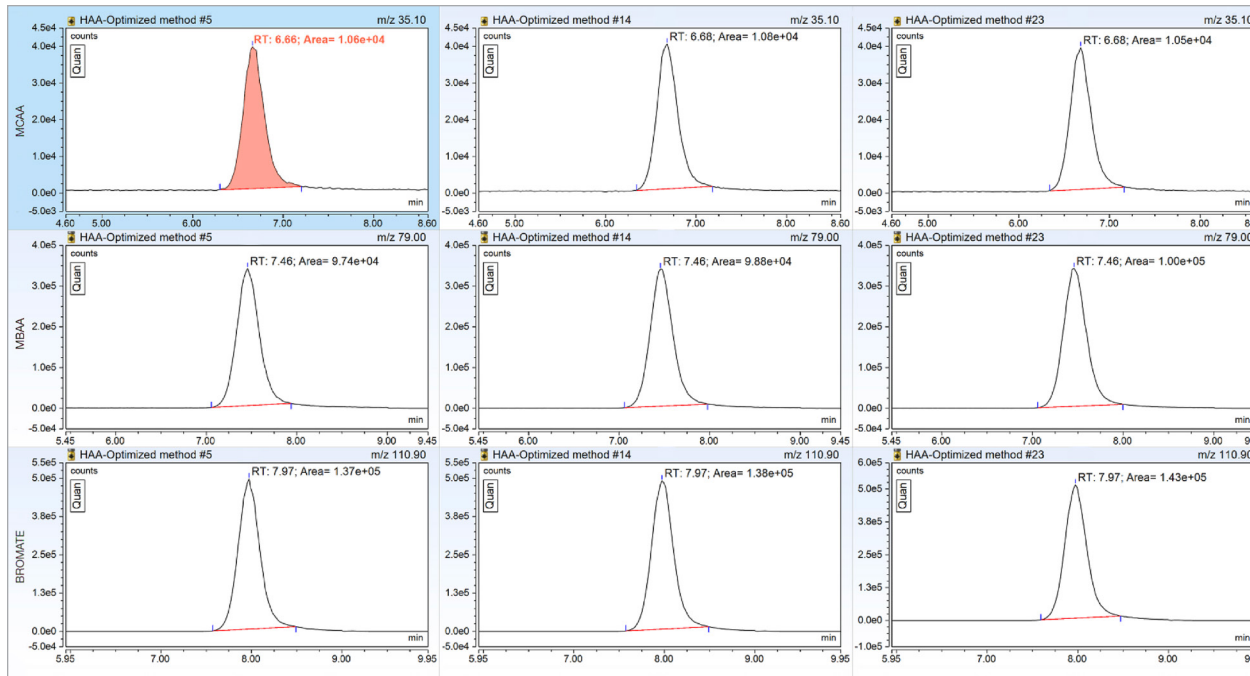


Nine HAAs, dalapon, and bromate eluted from the Dionex ICS-6000 HPIC system at 5 ppb in a 100 ppm  $\text{NH}_4\text{Cl}$  buffer (used as a preservative). Automatic injection into the TSQ Fortis mass spectrometer for MS/MS analysis provided excellent sensitivity.



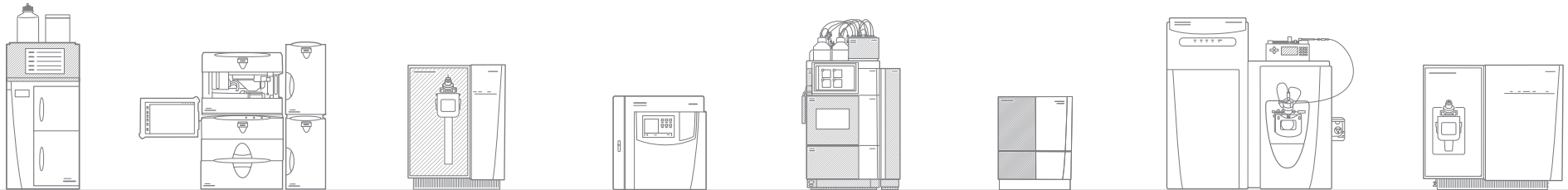
Ion chromatograms of three replicate injections of the HAA5, TCAA, bromate, and dalapon at 5 ppb in  $\text{NH}_4\text{Cl}$  buffer demonstrated excellent separation, sensitivity, and repeatability within 3%.

IC area peak repeatability of MCAA, MBAA, and bromate was within 10%. Sample injections for each were 5 ppb.



## Providing innovative chromatographic workflow solutions

Thermo Fisher Scientific offers a comprehensive portfolio of IC, GC, LC, and MS instruments to help you solve complex analytical challenges. Our leading-edge workflow solutions—from sample preparation, chromatographic separation, seamless integration with mass spectrometry, and data management and analysis help you meet today's increasing demands for analytical performance, productivity, and ease-of-use.



Thermo Scientific™  
Dionex™ Integrion™  
HPIC™ System

Thermo Scientific™  
Dionex™ ICS-6000  
HPIC™ System

Thermo Scientific™  
Orbitrap Exploris™ 240  
Mass Spectrometer

Thermo Scientific™  
TRACE™ 1310  
Gas Chromatograph

Thermo Scientific™  
Vanquish™  
HPLC System

Thermo Scientific™  
ISQ™ EC Single  
Quadrupole  
Mass Spectrometer

Thermo Scientific™  
Q Exactive™ HF  
Hybrid Quadrupole  
Mass Spectrometer

Thermo Scientific™  
TSQ Fortis™  
Triple Quadrupole  
Mass Spectrometer

Find out more at [thermofisher.com/HAAWorkflow](https://www.thermofisher.com/HAAWorkflow)

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