APPLICATIONS

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LC-HRMS Analysis of Haloacetic Acids (HAAs) and Dalapon in Water using a Luna® Omega Polar C18 3 µm 100 x 4.6 mm Column

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Overview

Haloacetic Acids (HAAs) are small polar contaminants in disinfected water. One major source for these molecules is the chlorination of drinking water. The respective synthetic pathways are supported by low pH conditions and high organic content in the water. Because of the negative health effects of HAAs when consumed over an extended period at elevated concentrations, their concentration in drinking water is regulated in various countries, and consequently must be monitored strictly.

The use of LC-MS/MS to determine HAAs in water has gained attention in recent years. This is linked to advances in LC column technology, that allowed the development of silica-based stationary phases with increased affinity for polar compounds like the Luna Omega Polar C18 used for this application.

In this application note we are presenting a LC-HRMS method for the effective monitoring of 13 HAAs and dalapon in drinking water.

Experimental Conditions

The analyses were performed on a SCIEX® ExionLC™ system equipped with a Shimadzu® FCV -11AL reservoir selection valve and 0.5 mL injection loop connected to a SCIEX X500R QTOF mass spectrometer.

HPLC Parameters

Column: Luna Omega Polar C18 3 µm
Dimensions: 100 x 4.6 mm
Part No.: 00D-4760-E0
Guard Column: SecurityGuard™ Polar C18 4 x 3 mm
Part No.: AJ0-7601
Mobile Phase: A: 0.1 % Formic acid in water
B: 0.1 % Formic acid in ACN
Gradient:

Time [min]	%B
0	5
3	5
5	20
7	100
10	100
11.5	5
16	5

Flow Rate: 1 mL/min
Injection: 200 µL acidified water sample (0.1% FA)
Detection: MSD

Mass Spectrometer Parameters

Mass acquisition was performed using negative electrospray ionization and a high resolution multiple reaction monitoring (MRM^{HR}) workflow.

Table 1. Ion Transitions and Compound Dependent Parameters

Analyte	TOF MS	Parent Ion	Fragment Ion	CE
Chloroacetic Acid (CAA)	92.9743	92.97	34.9693	-15
Bromoacetic Acid (BAA)	136.9238	136.92	78.9189	-15
Iodoacetic Acid (IAA)	184.9099	184.91	126.9050	-15
Dichloroacetic Acid (DCAA)	126.9353	126.93	82.9461	-10
Dibromoacetic Acid (DBAA)	216.8330	216.83	172.8430	-15
Diiodoacetic Acid (DIAA)	310.8070	310.81	266.8172	-10
Bromo-chloroacetic Acid (BCAA)	170.8848	170.88	78.9189	-25
Bromo-iodoacetic Acid (BIAA)	262.8204	262.82	126.9050	-35
Chloro-iodoacetic Acid (CIAA)	218.8709	218.87	126.9050	-20
Trichloroacetic Acid (TCAA)	116.9067	116.91	34.9693	-10
Tribromoacetic Acid (TBAA)	250.7536	250.75	78.9189	-20
Dichloro-bromoacetic Acid (DCBAA)	162.8540	162.85	78.9189	-10
Dibromo-chloroacetic Acid (DBCAA)	206.8034	206.80	78.9189	-15
2,2 Dichloropropionic Acid (DPN)	140.9511	150.95	34.9693	-25
2,3-Dibromopropanoic Acid (ISTD)		78.92	78.9192	-20

Table 2. MS Source Parameters

Source Parameter	Setting
Source Temp [°C]	650
Curtain Gas	Nitrogen
Curtain Gas Pressure [psi]	45
Ion Spray Voltage [V]	-3,500

Chromatograms and Retention Times

Table 3. Retention Times

Analyte	t_R	Analyte	t_R
CAA	2.4	CIAA	3.1
BAA	2.9	TCAA	4.2
IAA	4.6	TBAA	6.5
DCAA	2.0	DCBAA	4.8
DBAA	2.7	DBCAA	5.7
DIAA	6.5	DPN	4.3
BCAA	2.3	ISTD	7.7
BIAA	3.9		

Figure 1a. Tap water fortified with only Cl containing HAAs

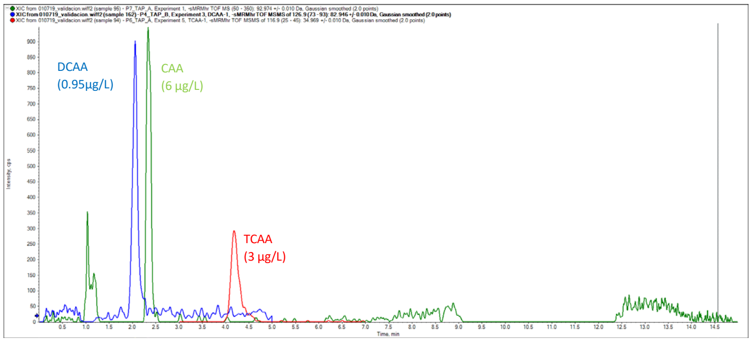


Figure 1b. Tap water fortified with only Br containing HAAs

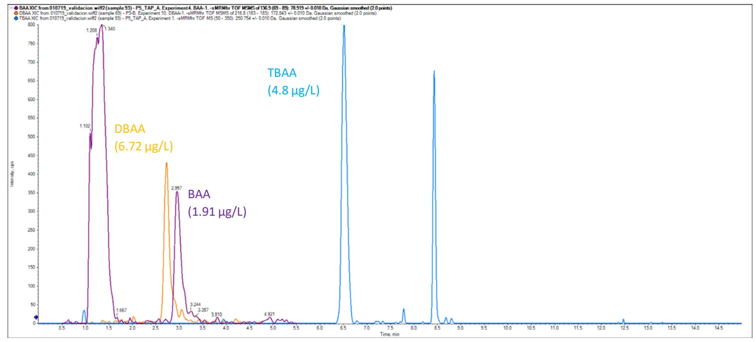


Figure 1c. Tap water fortified with I containing HAAs

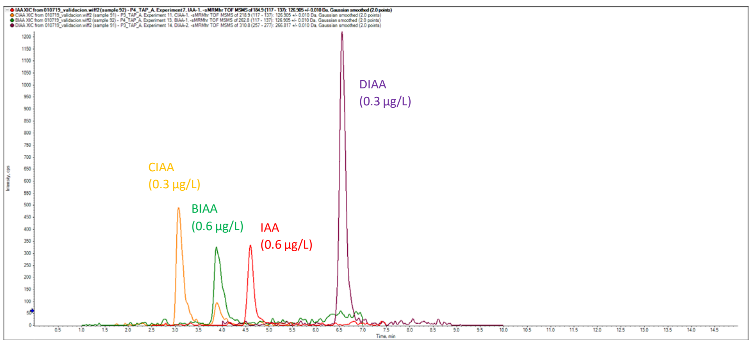
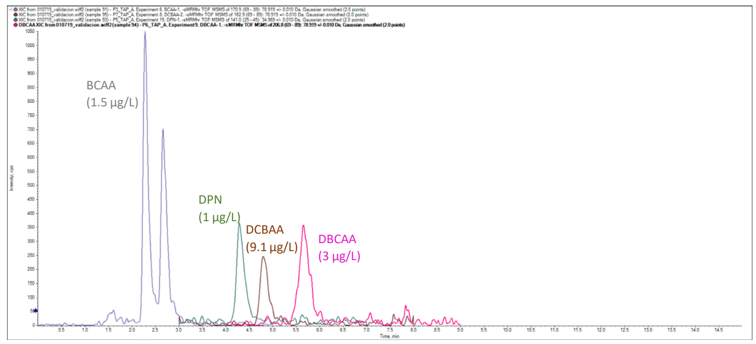


Figure 1d. Tap water fortified with dalapon and Br and Cl containing HAAs



Results and Discussion

The presented reversed phase method allows a fast and reliable quantification of HAAs in drinking water samples under gradient conditions. The use of the Luna Omega Polar C18 phase provides the retention required to minimize ion suppression effects. Therefore, it is possible to inject the water samples directly with only a minimal sample pretreatment (internal standard addition and acidification). No sample extraction process is needed to monitor these compounds at concentrations below the regulated levels. The column used for this study has been used for the analysis of 480 injections of various waters including fortified tap water, groundwater and surface water without any loss of separation performance.

Acknowledgements

Special thanks to Cristina Postigo at the Institute of Environmental Assessment and Water Research in Barcelona for contributing this method.

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