

# Simultaneous Detection of Haloacetic Acids using Ion Chromatography

## Electrospray Ionization Tandem Mass Spectrometry

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### Introduction & Objective

#### Context and Background:

- Haloacetic acids (HAAs) are a group of disinfection byproducts that has caused concern due to its potential harmful effects from long term exposure.
- HAAs are especially concerning when the drinking water source is linked with water reuse, which typically involves multiple forms of disinfection.
- Typical forms of detection are time consuming and allow for possible analyte loss.
- HAAs are moderately strong acids in drinking water (pH >6) and disassociate to haloacetate ions, making them suitable for ion chromatography.

#### Objective:

- Detection of HAAs in drinking water through ion chromatography, negative-ion electrospray ionization tandem mass spectrometry through direct injection and without the need for extraction and concentration.

### Mass Spectrometer Acquisition Conditions

Mass Spectrometer: Agilent 6490 MS/MS

#### Source Parameters:

- Gas Temperature: 120°C
- Gas Flow: 13 l/min
- Nebulizer: 45 psi
- Sheath Gas Temperature: 390°C
- Sheath Gas Flow: 12 l/min
- Capillary: 3000V
- Nozzle Voltage: 1500V
- Chamber Current: 0.24 μA

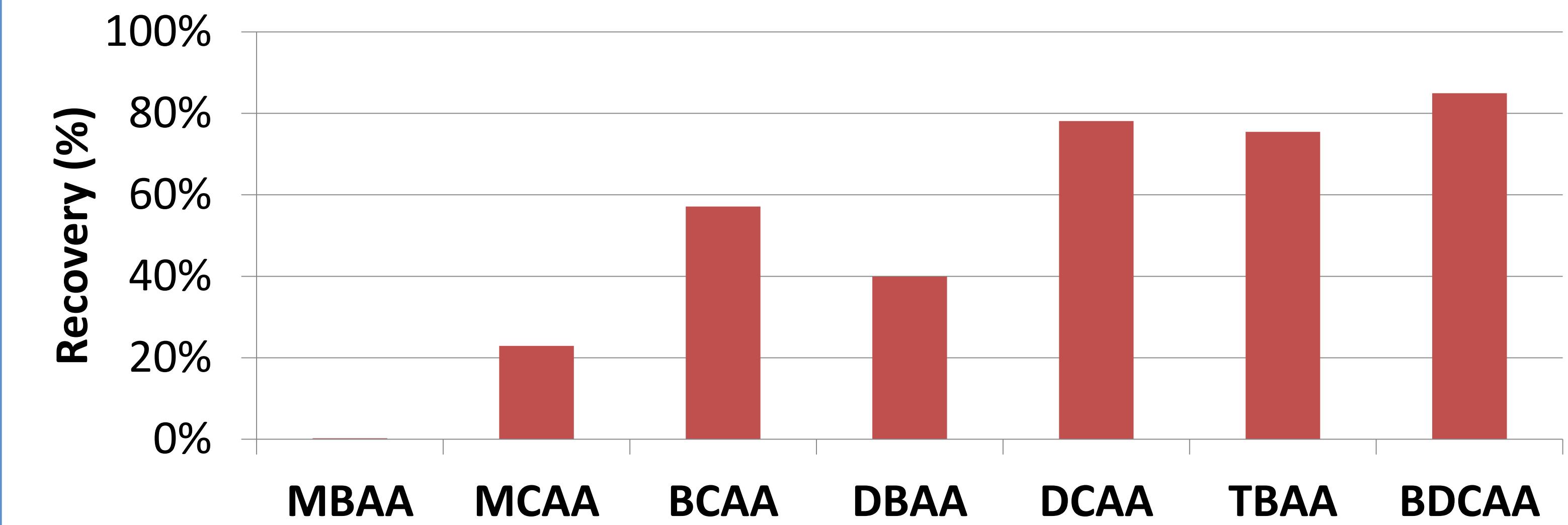
#### iFunnel Parameters:

- High Pressure RF: 160 V
- Low Pressure RF: 40

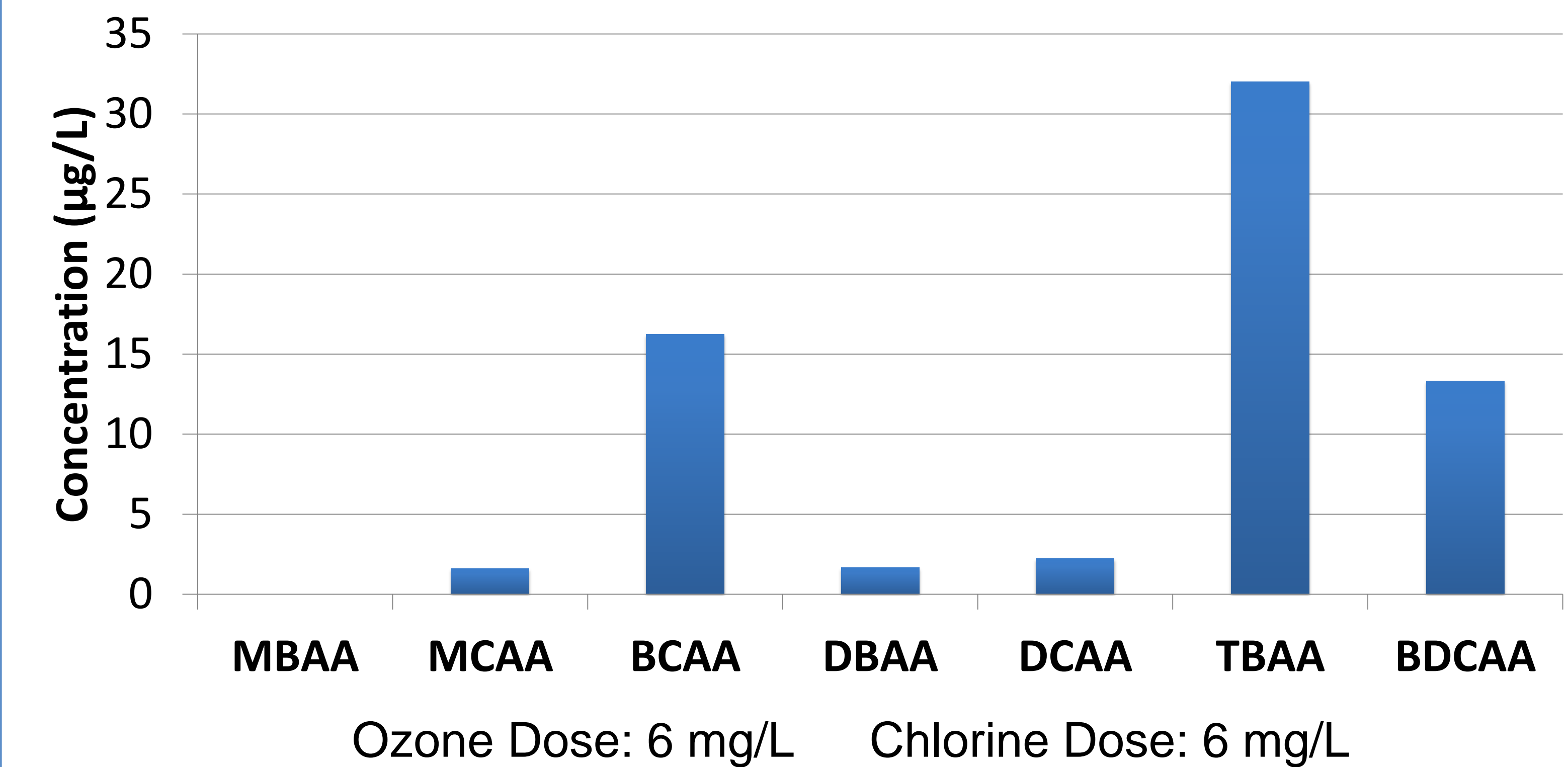
Compound Name	Precursor Ion	Product Ion	Collision Energy
Monobromoacetic Acid (MBAA)	137	83	6
Monochloroacetic Acid (MCAA)	93	35	6
Bromochloroacetic Acid (BCAA)	173	128.9	8
Dibromoacetic Acid (DBAA)	216.8	173	8
Dichloroacetic Acid (DCAA)	127	83	6
Tribromoacetic Acid (TBAA)	250.9	78.9	20
Bromodichloroacetic Acid (BDCAA)	163	81	8

### Waste Water Sample Results

#### True Recovery (%) of HAAs in Waste Water



#### HAAs in Ozonated and Chlorinated Waste Water



### Ion Chromatographic Conditions

**Ion Chromatography System:**  
Metrohm 850 Professional IC Anion

**Injection Volume:** 150 μL

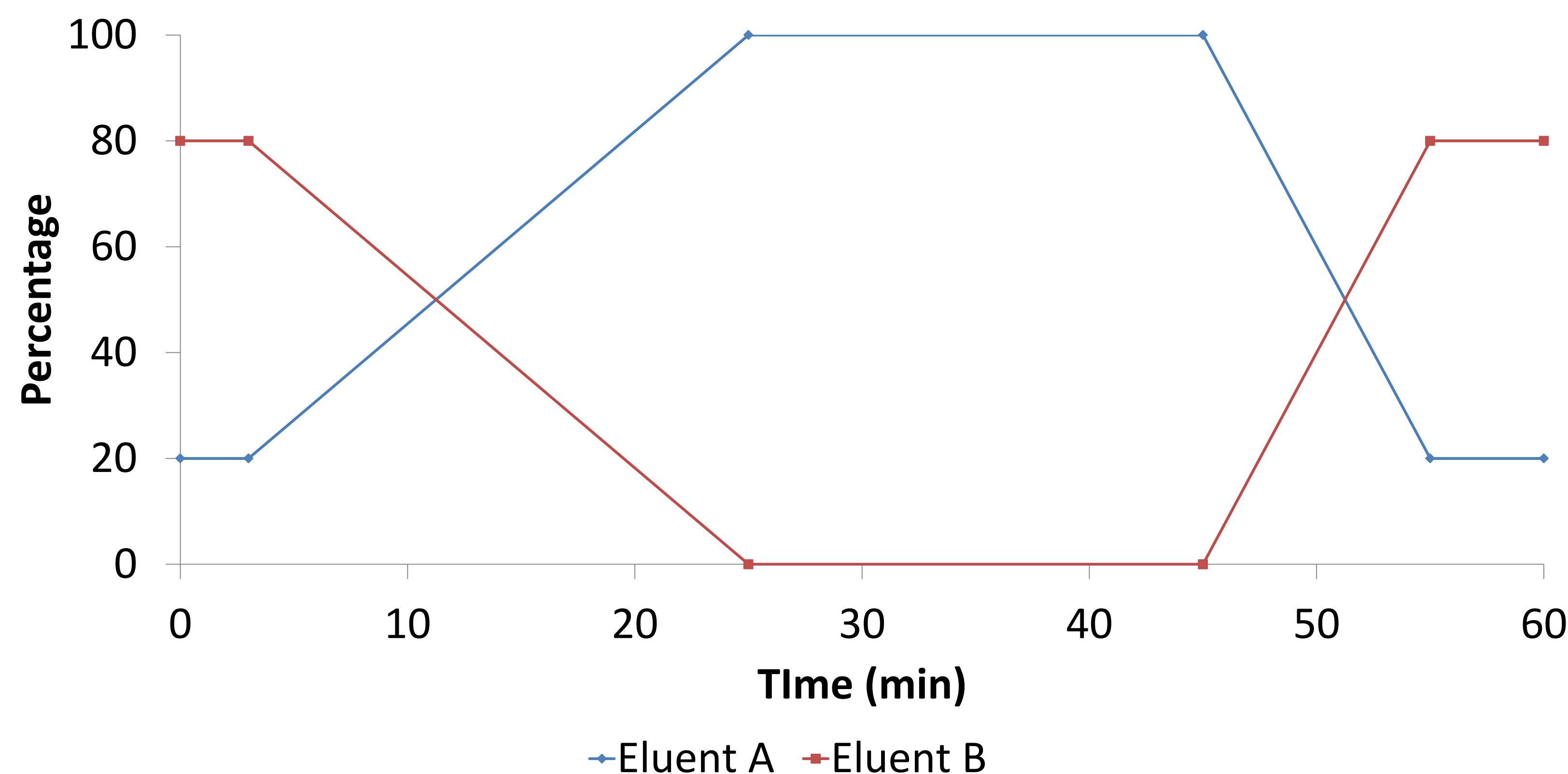
**Column:** Metrosep A Supp 7  
250mm x 4mm

**Eluent Flow Rate:** 0.4ml/min

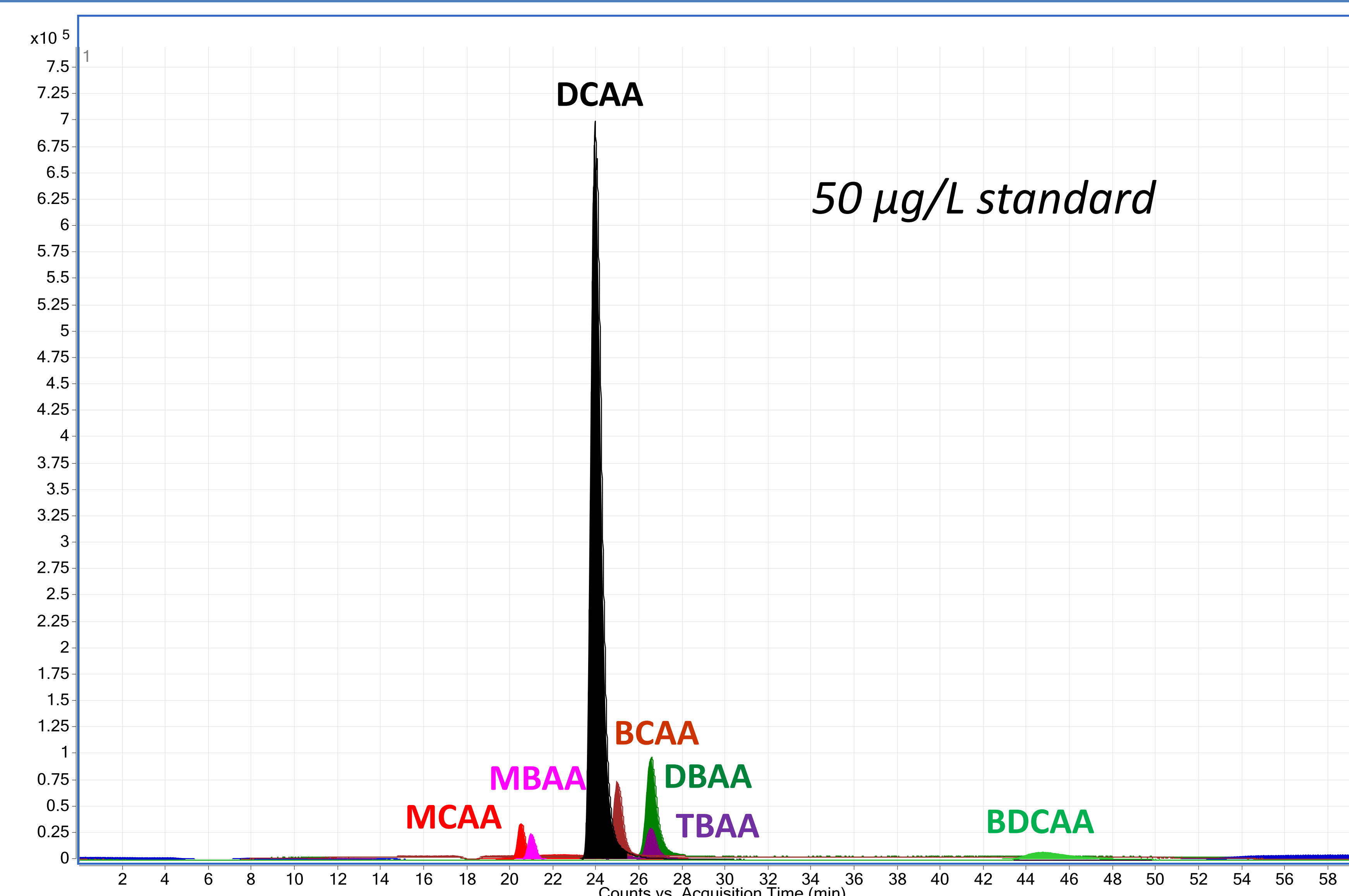
**Eluents:** A: 100mM NaOH  
B: 5% Acetonitrile

**Column Temperature:** 20°C

#### Eluent Gradient



### Chromatogram Results



### Conclusion

- Successful detection of seven HAAs. Future method development must be made to account for missing HAAs.
- Use of isotopically labeled standards is suggested due to low recoveries in wastewater.
- Direct injection allows for easier determination by eliminating necessary derivatization and extraction typically needed in other HAAs detection methods.

### Acknowledgment

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