Sensitive and Reliable Analysis of N-Nitrosamines in Water by Isotope Dilution GC-Tandem MS using the Agilent 7000B Triple Quadrupole GC/MS in EI Mode

ENVIRONMENTAL ANALYSIS

The Agilent 7000B Triple Quadrupole GC/MS enables MDLs as low as 0.4 ng/L for 8 N-nitrosamines in a variety of water sources

A wide range of disinfection processes used in water treatment plants can generate N-Nitrosamines. Laboratory animal studies have linked exposure of these compounds to cancers. Some nitrosamines have been classified by national and international regulatory authorities as probable human carcinogens. Regulation of N-nitrosamines in drinking waters is rapidly increasing in many parts of the world. Guidelines set by the World Health Organization and Australia call for a guideline of 100 ng/L for NDMA, and California has a notification level of 10 ng/L.

A GC/MS/MS method has been developed using the Agilent 7000B Triple Quadrupole GC/MS at the UNSW Water Research Center, Australia, for eight N-nitrosamines in drinking water and treated municipal effluent[1]. This Environmental Analysis describes the key performance parameters of the method; a copy of the full research report in the journal *Talanta* can be obtained from the Agilent web site.

Water samples are extracted by solid phase extraction (SPE) and then analyzed by GC/MS/MS. The use of direct isotope analogues for isotope dilution analysis of all analytes ensures accurate quantification, accounting for analytical variabilities that may occur during sample processing, extraction and instrumental analysis. The MDLs for all analytes were 0.4–4 ng/L in a variety of aqueous matrices. Sample matrices were observed to have only a minor impact on MDLs, and the method validation confirmed satisfactory method stability over intra-day and inter-day analyses of tap water and tertiary treated effluent samples, with coefficients of variation (σ/μ) as low as 0.03 and no higher than 0.08, inter-day.

The Agilent 7000B Triple Quadrupole GC/MS provides sensitivity, selectivity, and instrument stability to enable highly accurate, reproducible, and simultaneous determination of 8 N-nitrosamines, even in treated wastewater.

Key Benefits

- Accurate quantification using isotope dilution
- MDL of 0.81 ng/L in tap water for NDMA
- Intra-day and inter-day coefficients of variation (CVs) ≤ 9%, in treated wastewater
- An electron ionization (EI) method that does not require CI gases
- 14 minute analysis time and no derivatization required

1 J. A. McDonald, N. B. Harden, L. D. Nghiem, S. J. Khan "Analysis of N-nitrosamines in water by isotope dilution gas chromatography-electron ionisation tandem mass spectrometry", *Talanta* 99, 146-154 (2012).

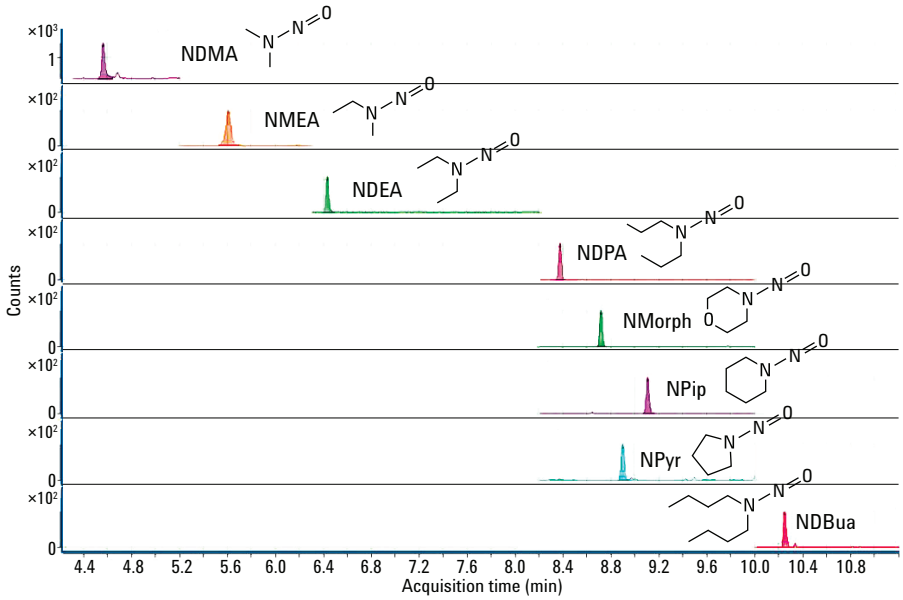

Figure 1. Chromatogram showing quantifier peaks for all eight nitrosamines at 1 pg on column.

Table 1. Instrument Detection Limits (IDLs) and Method Detection Limits (MDLs) of Target Analytes in Three Water Matrices

Analyte	IDL pg (on column)	Ultrapure water MDL ($ng.L^{-1}$) n = 7	Tap water MDL ($ng.L^{-1}$) n = 7	Tertiary treated effluent MDL ($ng.L^{-1}$) n=7
NDMA	0.3	0.45	0.81	*
NMEA	0.3	0.55	0.64	0.9
NDEA	0.1	0.94	0.83	*
NDPA	0.1	0.83	0.96	2.7
NMorph	0.3	0.67	0.43	*
NPyr	0.9	1.16	1.50	4.0
NPip	0.2	0.91	0.67	*
NDBuA	0.2	1.66	1.14	*

Injection volume is 1 µL, thus 1 ng/L is equal to 1 pg on column.

* MDLs for these compounds in tertiary treated effluent were unable to be determined due to background levels in this matrix.

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Published in USA, March 4, 2013
5991-1818EN

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