J Chromatogr Sep Tech 2017, 8:3(Suppl)
DOI: 10.4172/2157-7064-C1-026

Determination of low-ng/L level N-dimethynitrasamine in water by SPE-HPLC MS/MS

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N-nitrosodimethylamine (NDMA), were identified as chloramination byproducts in drinking water. NDMA are known as rodent carcinogens and probable human carcinogens, and so they are considered disinfection byproducts (DBPs) of public health concern. Several analytical techniques have been investigated for analysis of NDMA in water samples, including LC combined with UV detection, chemiluminescence (CL) combined with LC-UV, high-field asymmetric waveform ion-mobility spectrometry (FAIMS)-MS, HPLC-ion exclusion-UV-vis. However, the determination of low-ng/L level NDMA is not accurate. NDMA are typically detected in drinking water at low-ng/L concentrations, demanding highly sensitive analytical techniques to monitor and control them. A solid-phase extraction (SPE) ultra-high-performance-liquid chromatography coupled to a triple quadrupole mass spectrometer (HPLC–MS–MS) equipped with APCI ionization source method was established to determine the concentration of NDMA in water. The experiment results showed that APCI was able to better realize the ionization of NDMA and six other N-nitroamine than ESI. In MRM acquisition mode, ion of m/z 75.1 was determined as precursor ion in which product ion of m/z 58.2 and 43.3 were determined as qualitative and quantitative ions. The relative coefficient of standard curve (1-50μg/L) is 0.996 with pure water as solvents. The recovery rate is more than 80% and the method of determination (MOD) is 1.12-3.11 ng/L when water samples were concentrated by 400 times with coconut active charcoal as adsorbent. This method was applied to determine the concentration of NDMA for source water and treated water. The concentration of source water is lower than LOD. The average concentration of NDMA for treated water in Shanghai water source is 10.65-12.02 ng/L without significantly seasonal change which is probably related to PAM dosage. The successful determination of NDMA by LC MS/MS provides a new method for low-ng/L level NDMA as a supplement.

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Absolute cross sections for electron ionization of DNA and RNA bases

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Electron ionization cross sections of biological molecules are essential for modeling radiation damage so that accurate dosages of radiation can be applied in radiation therapy. However, reliable experimental data for many molecules are hardly available and obtaining theoretical data is difficult due to inherent complexity involved in modeling the process. In this context, we have developed a modified relative flow technique to obtain accurate partial and total ion cross sections by electron impact on molecules in solid form and with relatively low vapor pressure at room temperature. We have used this technique to obtain benchmark absolute partial and total ionization cross sections by electron impact on DNA and RNA bases and several other molecules of biological importance. The measurement techniques, the highlights of the cross section data and their comparison to the various theoretical calculations will be presented at the meeting.

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