

Determination of N-nitrosodimethylamine (NDMA) in drinking water by LC-MS/MS in Campinas, SP, Brazil.

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Abstract

N-Nitrosodimethylamine (NDMA) is a member of a family of extremely potent carcinogens, the N-nitrosamines. Current concern focuses on NDMA as a drinking water contaminant resulting from reactions during disinfection steps. The main purpose of this project is to evaluate NDMA levels on drinking water in the city of Campinas, SP.

Key words:

NDMA, Drinking water, Desinfection By-Product.

Introduction

N-Nitrosodimethylamine (NDMA) belongs to the N-nitrosamine family, with general moiety N-N=O as characteristic structure. N-nitrosamines form a group of genotoxic emergent chemicals, classified by International Agency for Research on Cancer (IARC) as probable human carcinogens¹. Since the 1950s, NDMA was found in food and consumer products as a result of unintended reactions between nitrites (preservatives) and amines^{2,3}. However, over the last few decades NDMA gained attention once again as it was detected as a Disinfection By-Product (DBP), produced by complex reactions between disinfection oxidants and organic matter naturally present in water⁴. So far, the maximum contaminant level (MCL) for NDMA in drinking water has not been established yet, though researchers agree it revolves around 3-10 ng. L⁻¹⁴. Given its relevance, the purpose of this project was to determine NDMA levels on drinking water samples in the city of Campinas, SP.

Results and Discussion

Determination of NDMA in drinking water used as guideline the USEPA method number 521⁵. A step of pre-concentration was required, employing Solid Phase Extraction (SPE) technique with extraction cartridges packed with coconut charcoal commercially available (Restek #26032). The analysis was performed with Liquid Chromatography coupled with tandem Mass Spectrometry LC-ESI(+)-QqQMS/MS (Agilent Technologies) with Zorbax SB-C18 column (2,1x30 mm, 3,5 µm) at a temperature of 27°C, mobile phase of 50:50 H₂O:MeOH + 0,1% (v/v) formic acid and a flow rate of 0,3 mL min⁻¹ in isocratic elution. NDMA quantification used Multiple Monitoring Reaction (MRM), monitoring precursor-product transition of 75-43 (m/z ± 0,1). The nebulizer pressure and radio frequency voltage were set in 35 psi and 4000 V, respectively.

Preliminary studies resulted in a limit of detection of 40 ng L⁻¹ and a recovery of 79,3% for synthetic samples. The average concentration of NDMA in drinking water treated conventionally was 2 µg L⁻¹. Next steps include determination of the compound in drinking water samples from alternative disinfection treatments and optimization of parameters for LC-MS/MS.

Image 1 shows the calibration curve obtained and Chart 1 shows the analytical parameters for NDMA analysis with LC-MS/MS.

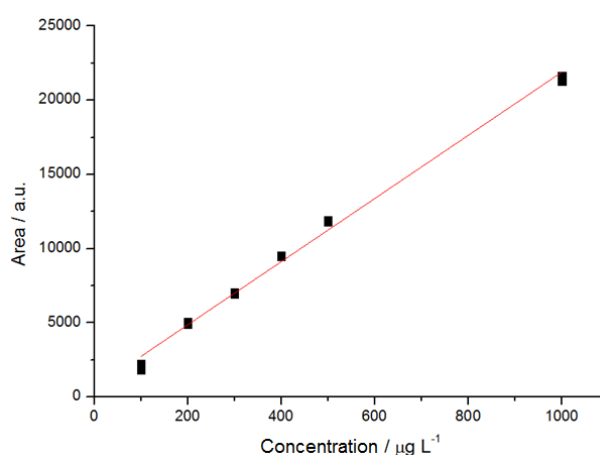


Image 1. Calibration curve for NDMA, with Pearson Correlation Coefficient of $R^2 = 0,99748$.

Chart 1. Analytical parameters for NDMA.

Parameter	Results
Mass	74,08 g mol ⁻¹
Retention time	0,45 min
Run time	1,45 min
Precursor ion	75,0 ± 0,1 m/z
Fragmentor	100 V
Quantification ion Q	43,0 ± 0,1 m/z
Collision energy of Q	15 eV
Confirmation ion C	58,2 ± 0,1 m/z
Collision energy of C	10 eV
Limit of quantification	40 ng L ⁻¹

Conclusions

Preliminary studies lead to believe that NDMA levels in drinking water samples from Campinas are higher than the suggested MCL of 3-10 ng L⁻¹, which reinforces research on alternative water disinfection treatments.

Acknowledgements

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¹ IARC, *Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans*, **1978**, 17, 365.

² Department of Health and Human Services, *Report on Carcinogens*, **2014**, 13th report.

³ Sharpley, D., *Science*, **1976**, 191, 268.

⁴ Mitch, W. A. et al., *Environmental Engineering Science*, **2001**, 20, 5.

⁵ Munch, J. W; Bassett M. V., *United States Environmental Protection Agency Document # EPA/600/R-05/054*, **2004**.