SUPPLEMENTARY INFORMATION

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Investigations into alternative analytical approaches for *N*−nitrosamine contamination in drinking water

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Table S1: Accurate masses used to extract *N*-nitrosamines from the total ion chromatograms obtained by UPLC-QToFMS analysis. The structures of the NAs and molecular weights (MW) are provided.

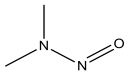
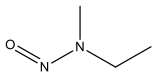
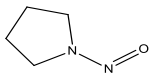
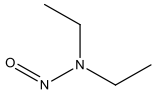
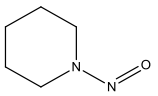
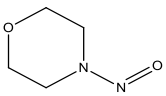
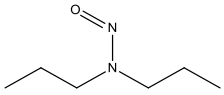
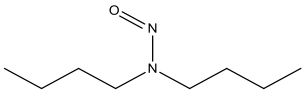
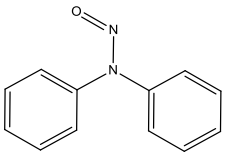
Name	Acronym	MW (g/mol)	Accurate Mass (+1) (g/mol)	Structure
***N*-nitrosodimethylamine**	NDMA	74	75.0550	
***N*-nitrosomethylethylamine**	NMEA	88	89.0715	
***N*-nitrosopyrrolidine**	NPyr	100	101.0715	
***N*-nitrosodiethylamine**	NDEA	102	103.0871	
***N*-nitrosopiperidine**	NPip	114	115.0871	
***N*-nitrosomorpholine**	NMor	116	117.0664	
***N*-nitrosodi-n-propylamine**	NDPA	130	131.1184	
***N*-nitrosodi-n-butylamine**	NDBA	158	159.1497	
***N*-nitrosodiphenylamine**	NDPhA	198	199.0871	

Table S2: UPLC-QToFMS parameters and conditions.

Parameter	Condition	
Column	Kinetex® 1.7 µm EVO C_{18} 100 Å (2.1 mm ID x 100 mm length)	
Ionization modes	ESI (+ / -)	APCI (+ / -)
Mobile phases	acetonitrile/ultrapure water methanol/ultrapure water	methanol/ultrapure water acetonitrile/ultrapure water
Analyzer	Resolution mode	
Source Temperature (ºC)	120	120
Sampling cone voltage (V)	25	25
Extraction cone voltage (V)	4	4
Cone gas (nitrogen) flow rate (L/hr)	10	10
Desolvation flow rate (L/hr)	300	300
Probe temperature (ºC)	20	
Corona discharge (µA)	5	

Table S3: GC-ToFMS parameters and conditions.

Parameter	Description
Column	RXi-1MS, 30 m length x 0.25 mm diameter x 0.25 µm film thickness
Carrier gas and flow rate (mL/min)	Helium, 1.00
Injection volume (µL)	1
Front inlet septum purge flow rate (mL/min)	3
Ion source temperature (ºC)	230
Acquisition rate (spectra/min)	10
Acquisition voltage (V)	1650
Electron energy (eV)	-70

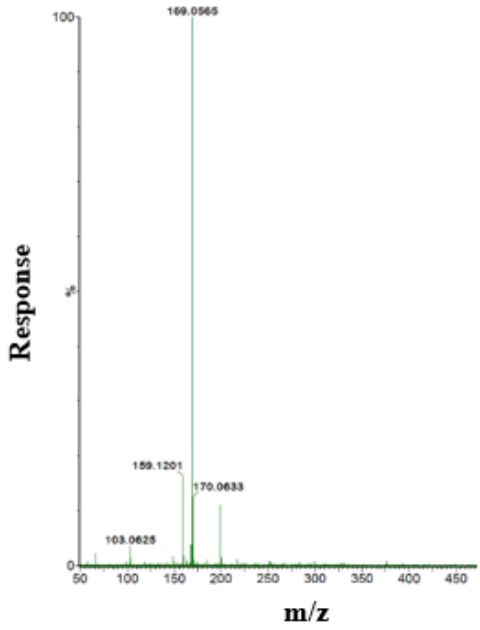


Fig S1: The mass spectrum of NDPhA showing the most abundant peak at m/z 169.06 obtained by UPLC-QToFMS analysis of a 5 µg/mL nitrosamine mix standard in methanol.

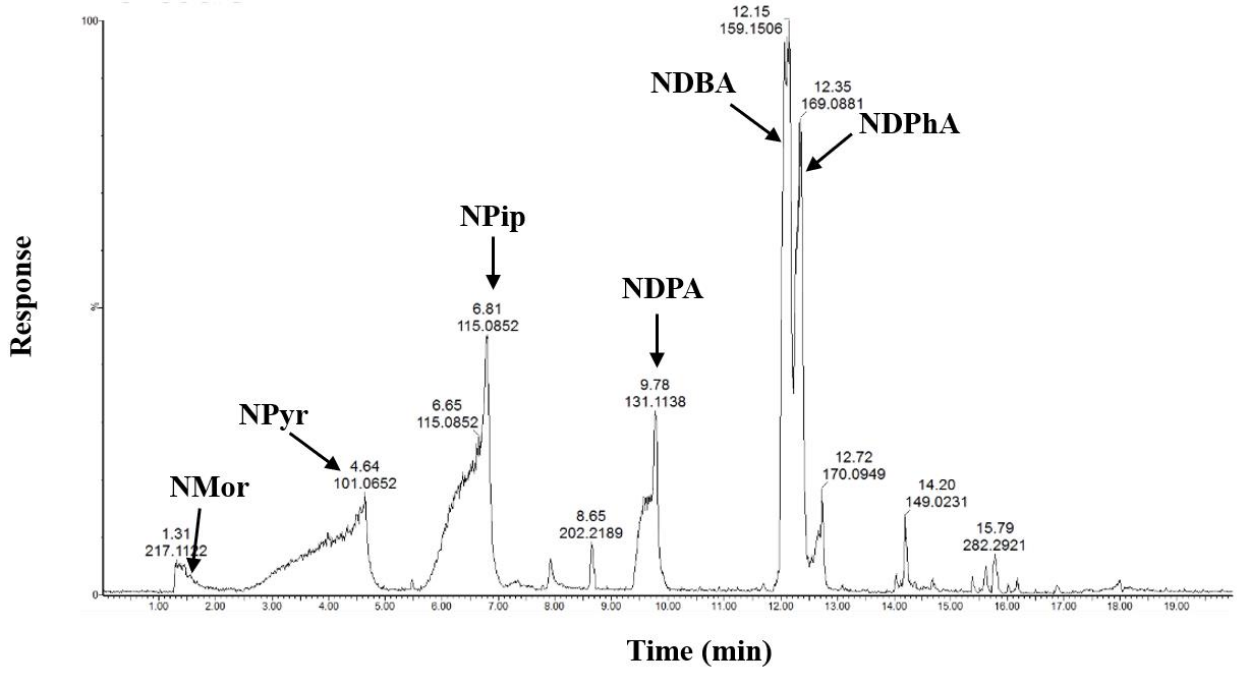


Fig S2: TIC of a 5 µg/mL nitrosamine mix standard in methanol analyzed by UPLC-QToFMS with APCI (+/-) using methanol/ultrapure water as a mobile phase. The injection volume was 30 µL using a 100 µL sample loop. Extensive peak broadening is noted when comparing this TIC to **Fig 1**.

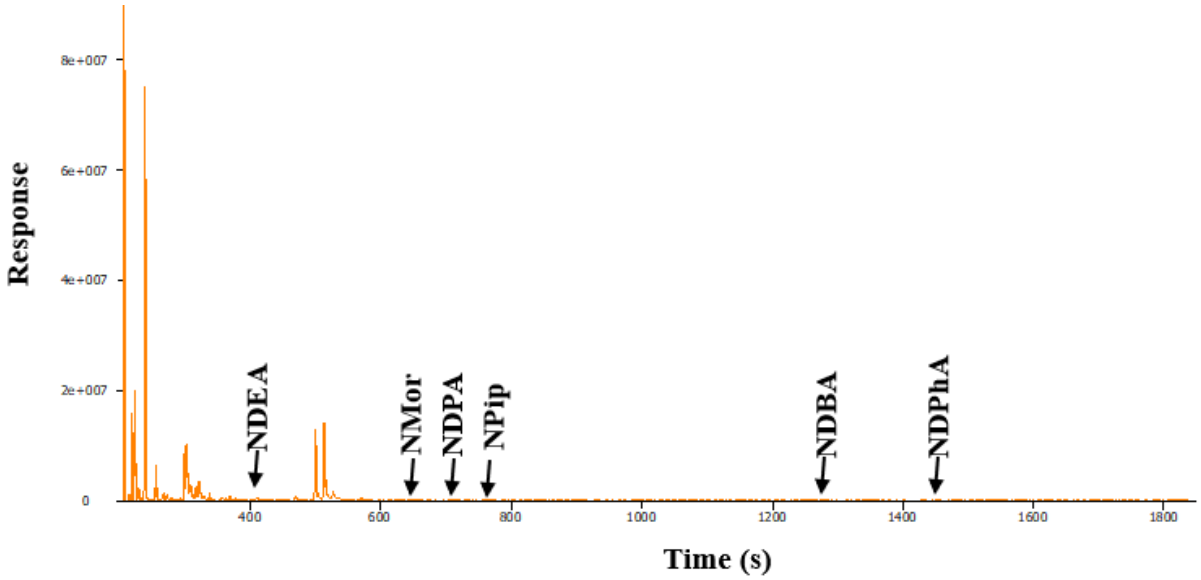


Fig S3: TIC of the nitrosamine mix standard (1 µg/mL) in hexane and acetone (9:1 v/v) analyzed by GC-ToFMS in splitless mode with 1 µL injection volume. Poor peak areas were observed and three NAs (NDMA. NMEA, and NPyr) were not detected.

Table S4: Percentages reflecting the change in peak areas of the respective NA analytes relative to that obtained on the first day of the stability analysis.

Analyte	% Area decreases between 9- 10 May	% Area decreases between 9-11 May	% Area decreases between 9-12 May	% Area decreases between 9-13 May	% Area decreases between 9-14 May	% Area decreases between 9-21 May
NDMA	32%	53%	70%	70%	66%	-16%
NMEA	-1%	42%	50%	53%	60%	-16%
NDEA	20%	50%	65%	62%	70%	8%
NPyr	47%	60%	83%	61%	74%	17%
NMor	18%	60%	64%	68%	69%	10%
NDPA	20%	52%	67%	66%	67%	17%
NPip	24%	49%	66%	68%	69%	14%
NDBA	37%	78%	79%	80%	86%	18%
NDPhA	-39%	20%	11%	6%	31%	-164%
Average %	18%	52%	62%	59%	66%	-12%
% RSD	134.93	28.45	32.40	33.85	21.26	442.38

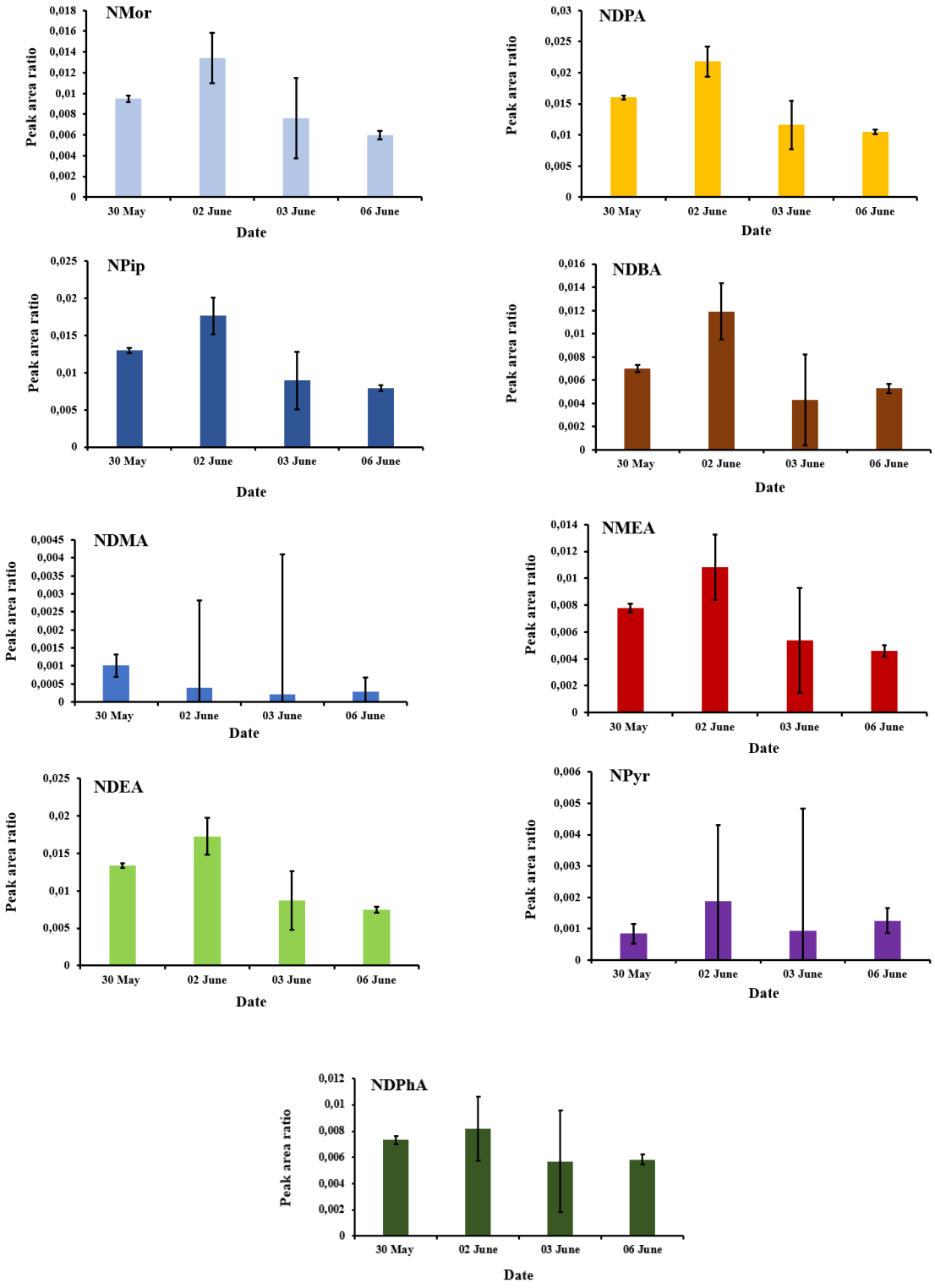


Fig S4: Individual peak area ratio (analyte/pyrene) over time for the nine NA analytes stored in 1.5 mL amber vials analyzed by GC-ToFMS (1 µL injection). Error bars represent the standard deviation of the peak area ratios. 5 µg/mL concentration for both the pyrene and analytes.