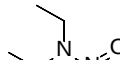
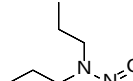
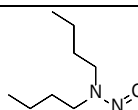
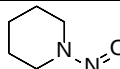


SUPPORTING INFORMATION TO:

DETERMINATION OF N-NITROSAMINES BY GAS CHROMATOGRAPHY COUPLED TO
QUADRUPOLE - TIME OF FLIGHT MASS SPECTROMETRY IN WATER SAMPLES

Benigno J. Sieira, Inmaculada Carpinteiro, Rosario Rodil*, José Benito Quintana, Rafael
Cela

Table S1. Structure and properties of the *N*-nitrosamines considered in this work

Abbreviation	Compound Name	CAS Number	Molecular Formula	Structure	Molecular Weight (g/mol)	Boiling Point (°C) ^a	pK _a ^a	log K _{ow} ^a
NDMA	<i>N</i> -Nitrosodimethylamine	62-75-9	C ₂ H ₆ N ₂ O		74.08	152	- 3.63	- 0.496
NMEA	<i>N</i> -Nitrosomethylethylamine	624-78-2	C ₃ H ₈ N ₂ O		88.11	163	- 3.39	- 0.014
NDEA	<i>N</i> -Nitrosodiethylamine	55-18-5	C ₄ H ₁₀ N ₂ O		102.14	176	- 3.14	0.523
NDPA	<i>N</i> -Nitrosodipropylamine	621-64-7	C ₆ H ₁₄ N ₂ O		130.19	206	- 3.18	1.542
NDBA	<i>N</i> -Nitrosodibutylamine	914-16-3	C ₈ H ₁₈ N ₂ O		158.24	116	- 3.14	2.561
NPIP	<i>N</i> -Nitrosopiperidine	68374-62-9	C ₅ H ₁₀ N ₂ O		114.15	219	- 3.18	0.438
NPYR	<i>N</i> -Nitrosopyrrolidine	930-55-2	C ₄ H ₈ N ₂ O		100.12	214	- 3.14	- 0.089
NMOR	<i>N</i> -Nitrosomorpholine	59-89-2	C ₄ H ₈ N ₂ O ₂		116.12	224	- 5.72	- 0.594

^a Data calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2018 ACD/Labs)

Table S2: Compilation of MDLs reported in the literature for the determination of nitrosamines in water

Reference Sample Preparation & Detection Techniques	1	2	3	4	5	6	7	8	9	10	11
	SPE GC-EI- Magnetic Sector	SPE GC-EI- MS/MS (TQ)	GC-PCI- MS/MS (IT)	SPE GC-EI- MS/MS (TQ)	SPE GC-PCI- MS/MS (IT)	SPE LC-ESI-MS/MS (Orbitrap)	SPE LC-ESI- MS/MS (QTRAP)	SPE GC-EI-MS (Q)	SPE GC-PCI- MS/MS (IT)	SPME GC-PCI- MS/MS (IT)	SPME GC-PCI- MS/MS (TQ)
NDMA	0.8	1.1	0.3	0.5	0.8	0.4	3.1	10	1.0	5	30
NMEA	0.6	1.8	0.3	0.6	1.4	0.9	2.4	Not avail.	1.9	4	90
NDEA	0.1	1.6	0.3	0.9	1.8	0.7	10.6	3	1.4	3	64
NDPA	0.2	2.3	0.3	0.8	1.6	0.8	0.2	Not avail.	1.4	2	59
NDBA	0.1	3.1	0.4	1.7	1.6	3.3	3.1	13	2.7	1	79
NPIP	0.1	2.2	0.7	0.9	1.4	0.1	0.9	4	1.1	5	59
NPYR	0.2	1.7	0.4	1.2	0.8	1.0	2.1	12	1.5	1	Not avail.
NMOR	1.7	1.9	Not avail.	0.7	1.4	0.2	0.2	7	0.8	4	138

LC: liquid chromatography; QTRAP: Linear Ion Trap; Q: quadrupole; TQ: Triple quadrupole

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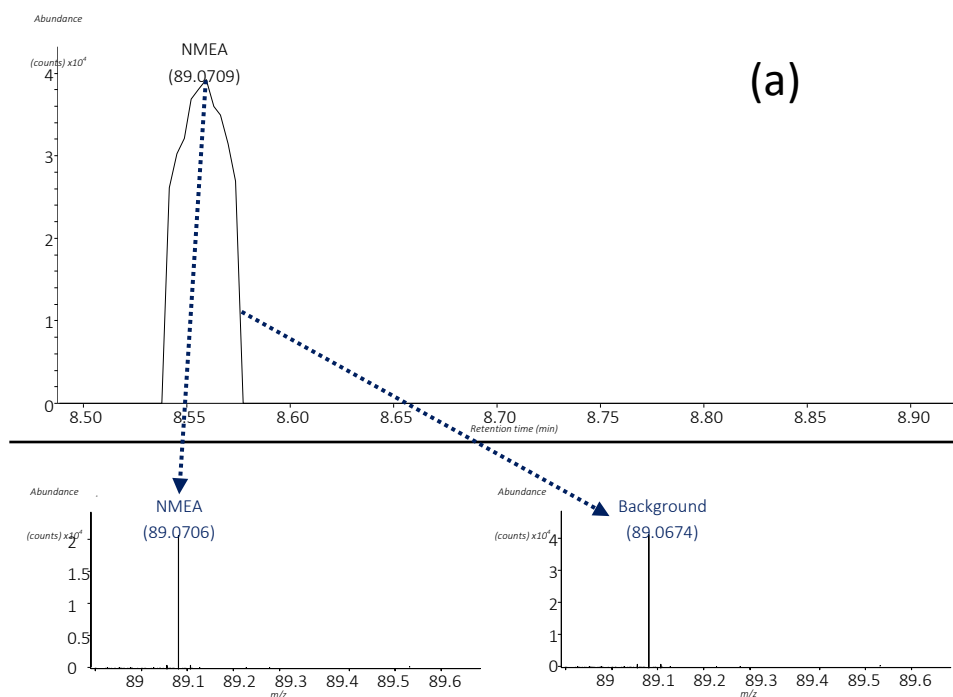
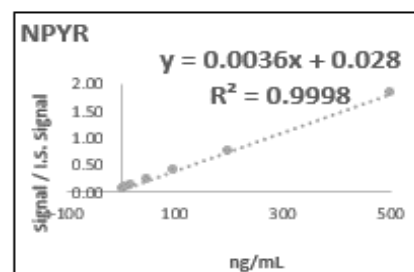
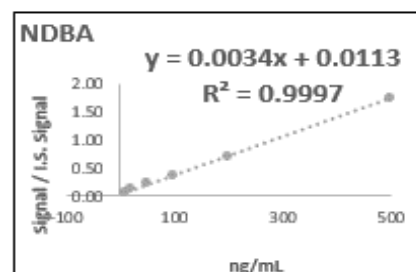
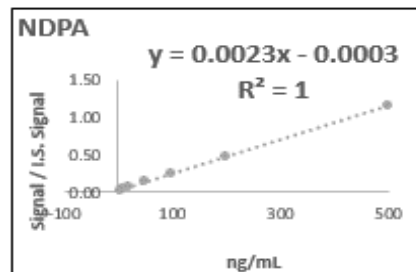
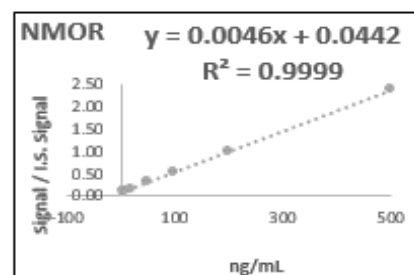
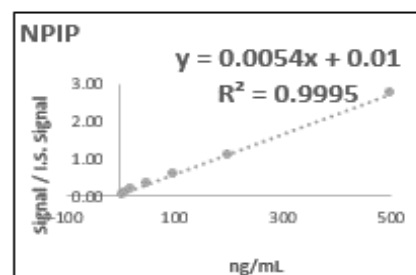
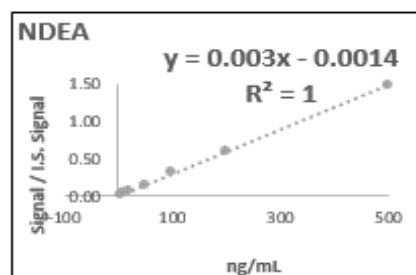
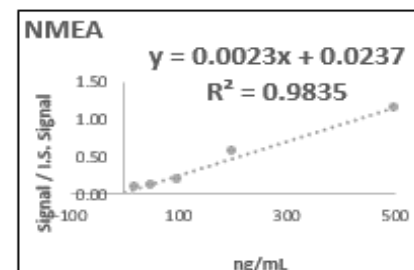
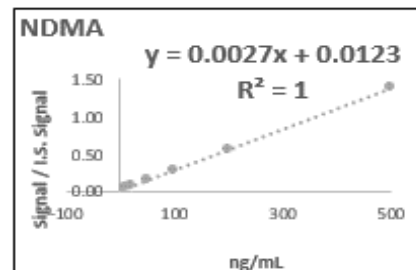
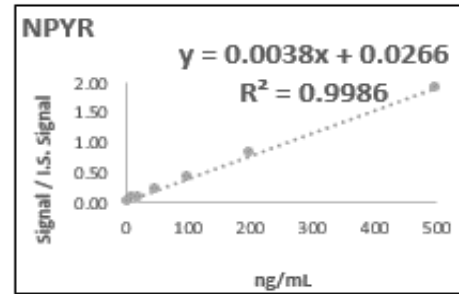
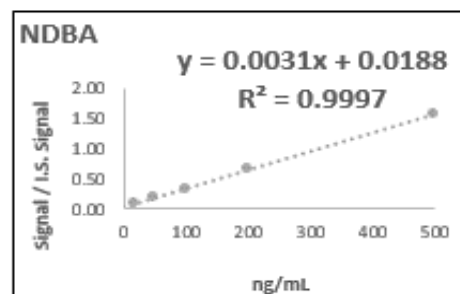
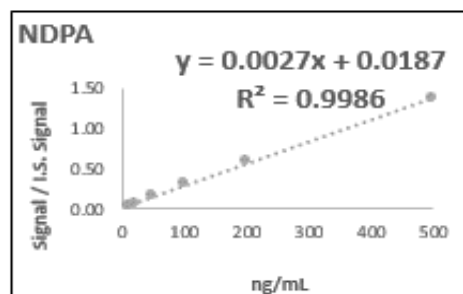
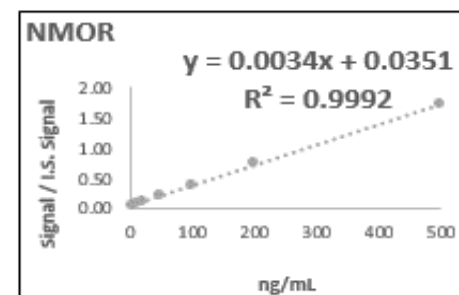
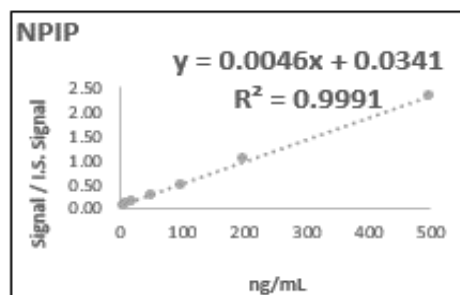
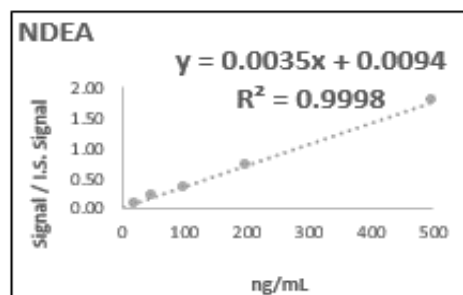
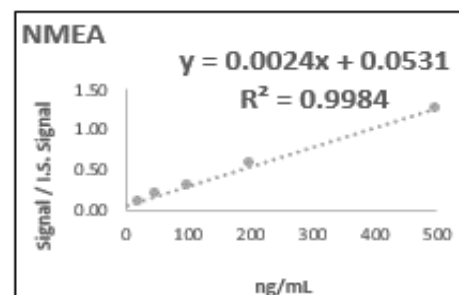
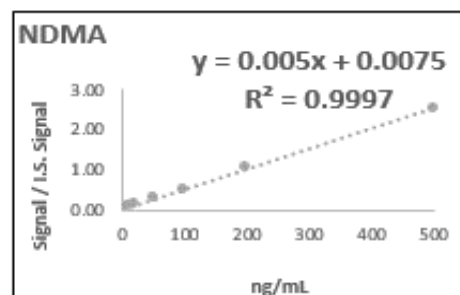


Figure S1. Isobaric interference for NMEA in PCI acquiring in centroid (A) and profile mode (B). Extracted ion chromatograms (EIC) with ± 50 ppm.

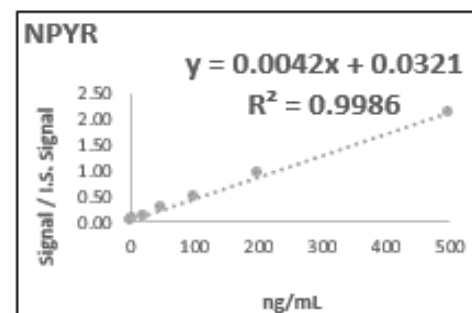
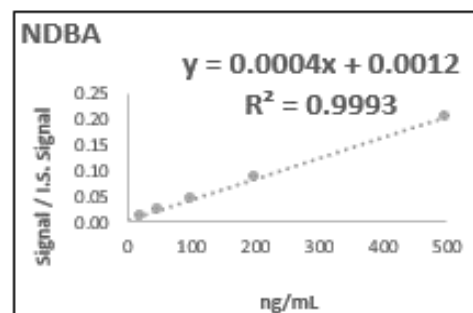
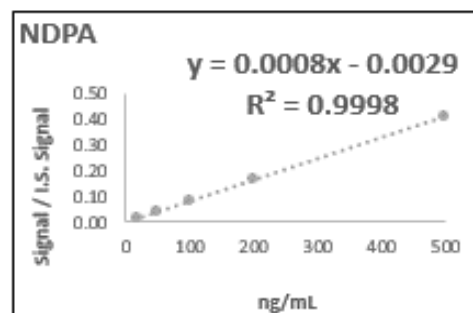
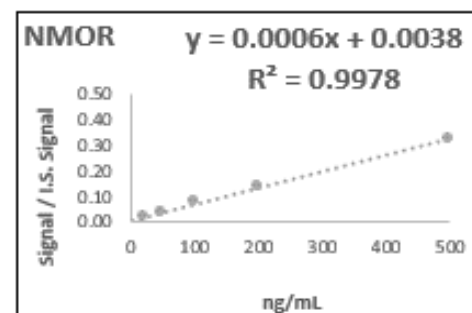
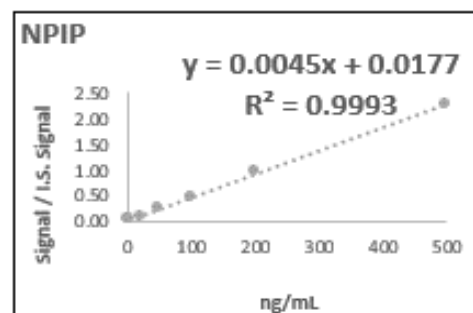
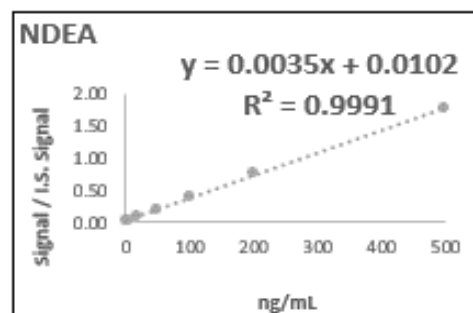
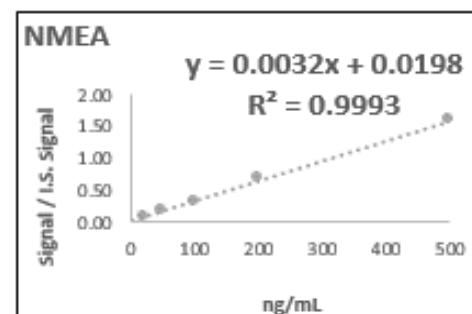
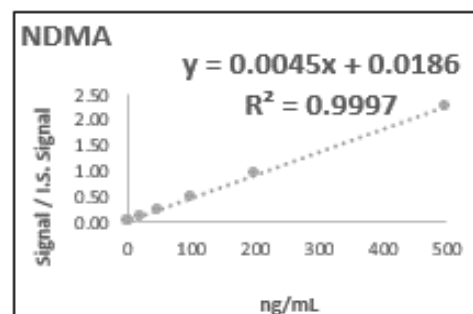
(a)



(b)



(c)



(d)

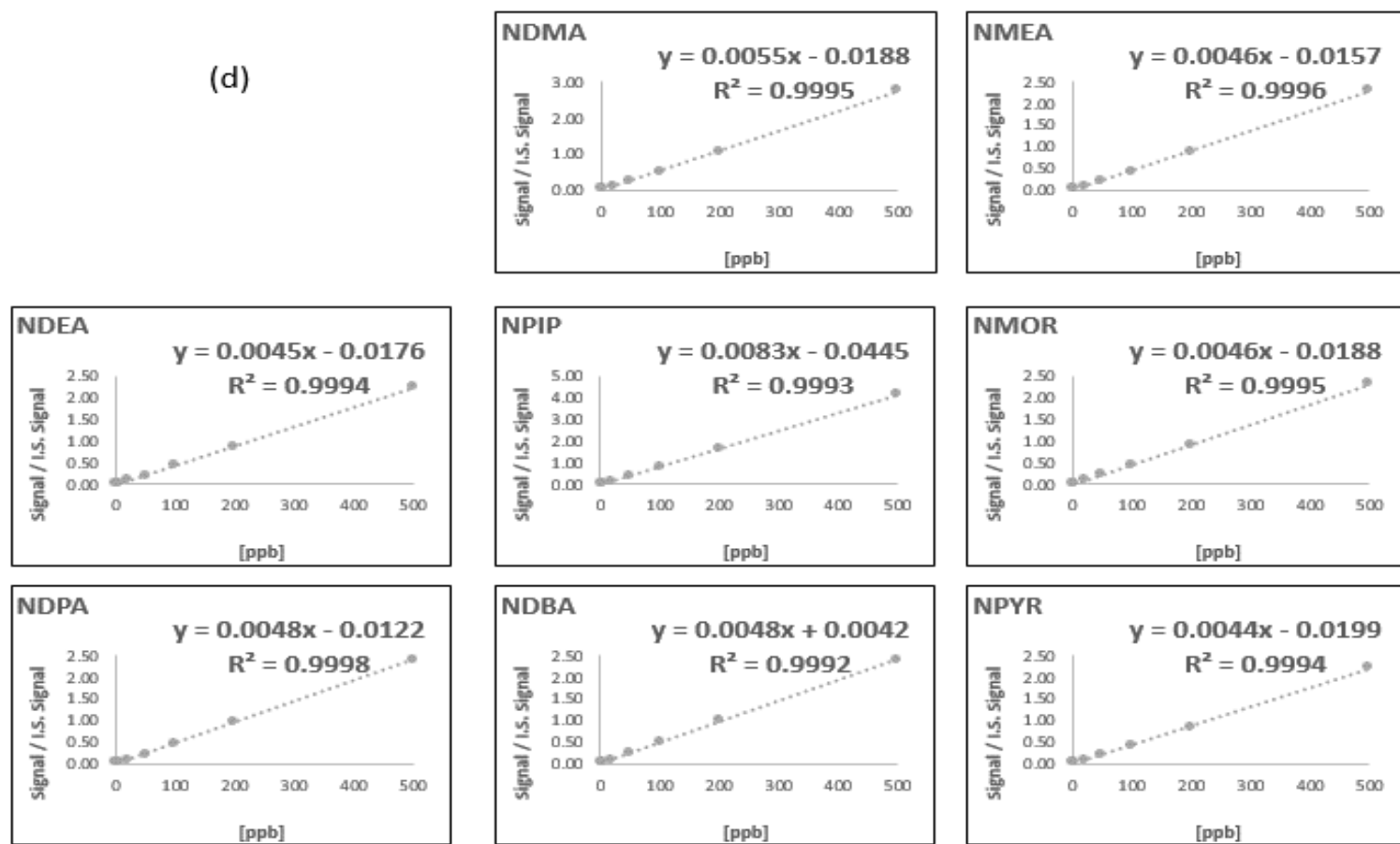


Figure S2: Calibration curves obtained by: (a) GC-EI—MS (IT), (b) GC-PCI—MS (IT), (c) GC-EI-MS (QTOF) and (d) GC-PCI-MS (QTOF)