

Supplementary Information

Monitoring *N*-Nitrosamines in Cosmetic Thermal Waters: Analytical Method Development, Validation, and Market Analysis in Brazil

*Maria Fernanda A. V. Matos,^a Gabriela F. P.de Souza,^a Anna Paula R.de Queiroga,^a
Airtton G. Salles Jr^b and Susanne Rath ^{*,a}*

^a*Departamento de Química Analítica, Instituto de Química, Universidade Estadual de Campinas,
13084-971 Campinas-SP, Brazil*

^b*Departamento de Química Orgânica, Instituto de Química, Universidade Estadual de Campinas,
13084-971 Campinas-SP, Brazil*

Table S1. Mass spectrometry conditions

Analyte	Abbreviation	PI (<i>m/z</i>)	QI (<i>m/z</i>) (CE / eV)	CI (<i>m/z</i>) (CE / eV)	Cone voltage / V
<i>N</i> -Nitrosodiethanolamine	NDELA	135	104 (5)	74 (10)	16
<i>N</i> -Nitrosodimethylamine	NDMA	75	58 (10)	43 (15)	30
<i>N</i> -Nitrosodiethylamine	NDEA	103	75 (10)	29 (15)	30
<i>N</i> -Nitrosomorpholine	NMOR	117	87 (10)	45 (13)	28
Internal standards (IS)	NDELA- <i>d</i> ₈	143	80 (11)	111 (5)	15
	NDMA- <i>d</i> ₆	81	46 (12)	64 (9)	23
	NDEA- <i>d</i> ₁₀	113	34 (11)	81 (10)	30
	NMOR- <i>d</i> ₄	121	61 (12)	91 (10)	22

PI: precursor ion; QI: quantitation ion; CI: confirmation ion; CE: collision energy.

*e-mail: rath@unicamp.br

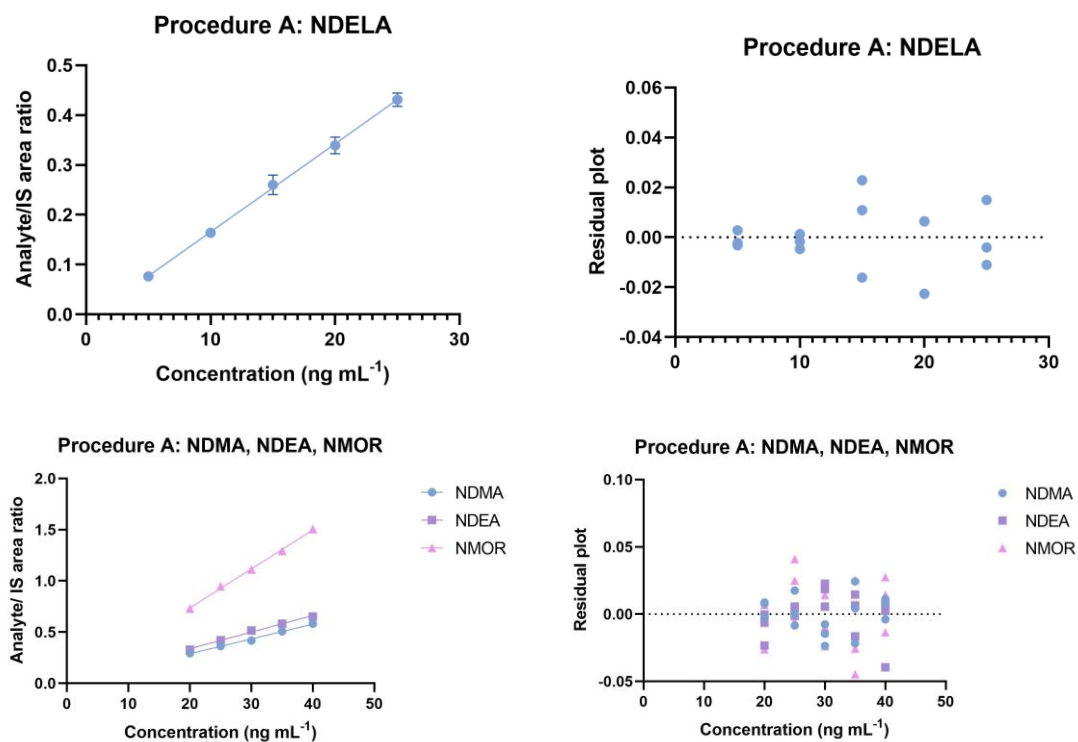


Figure S1. Internal standards calibration curves and corresponding residual plots for NDELA, NDMA, NDEA and NMOR using procedure A-direct injection and LC-LC-MS/MS.

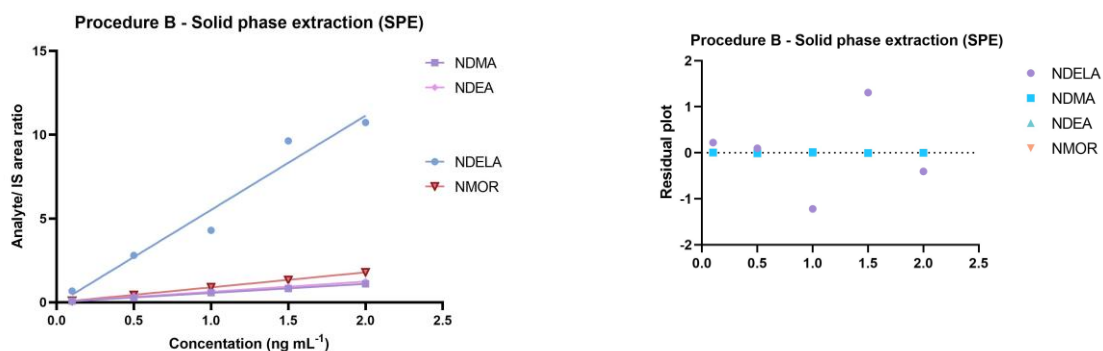


Figure S2. Internal standards calibration curves and corresponding residual plots for NDELA, NDMA, NDEA and NMOR using procedure B-solid phase extraction and LC-LC-MS/MS.

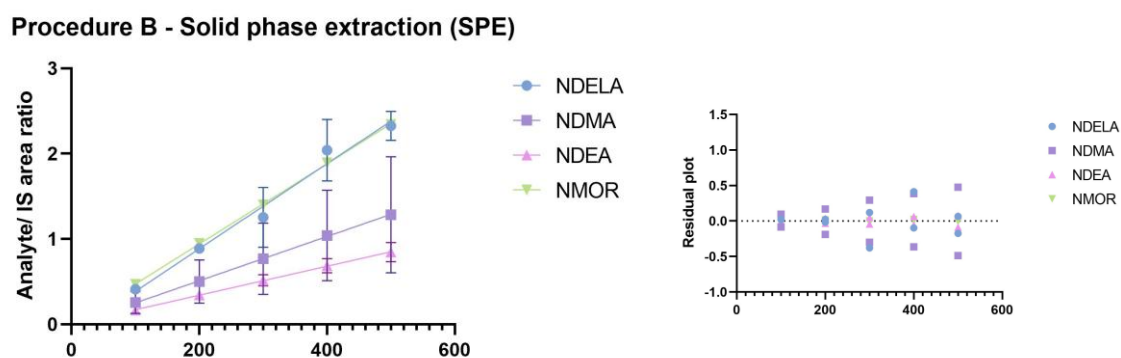


Figure S3. Internal standards calibration curves and corresponding residual plots for NDELA, NDMA, NDEA and NMOR using procedure B-solid phase extraction and LC-LC-MS/MS.