Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Determination of nine prohibited N-nitrosamines in cosmetic products by vortex-assisted dispersive liquid–liquid microextraction prior to gas chromatography-mass spectrometry

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Table S1. Box-Behnken design for multivariate optimization of the critical variables.

Step	$CHCl_3$ volume (µL)		Vortex time (s)		Ionic strength (%NaCl, w/v)	
	Uncoded	Coded	Uncoded	Coded	Uncoded	Coded
1	60	-1	60	0	0	-1
2	150	1	60	0	0	-1
3	60	-1	60	0	10	1
4	150	1	60	0	10	1
5	60	-1	30	-1	5	0
6	150	1	30	-1	5	0
7	60	-1	90	1	5	0
8	150	1	90	1	5	0
9	105	0	30	-1	0	-1
10	105	0	30	-1	10	1
11	105	0	90	1	0	-1
12	105	0	90	1	10	1
13	105	0	60	0	5	0
14	105	0	60	0	5	0
15	105	0	60	0	5	0

Box-Benhken design

Box-Benhken designs are a class of rotatable or nearly rotatable second-order designs used to generate high order response.

The total number of experiments required for the development of the Box-Benhken design (N) is defined by the following equation:

$$N = 2k(k-1) + Cp \quad (1)$$

where k is the number of factors (i.e., 3), and Cp is the number of replicates of the central point. In this sense, performing 3 replicates of the central point and according to Equation (1), 15 experiments were required. As shown in Table 3, the range of each factor was defined between a high and low value.

The following quadratic polynomial equation was applied to evaluate the multiple linear regression for each response:

$$Y = \beta_o + \Sigma \beta_i X_i + \Sigma \beta_{ii} X_i^2 + \Sigma \beta_{ij} X_i X_j + \varepsilon \quad (2)$$

where Y is the analytical response; β_0 is the constant term; β_i, β_{ii} and β_{ij} represent the regression coefficients of the design; χ_i and χ_j are the different variables; and ε is the residual error.

Afterwards, the global desirability of the experiment (D) was applied to study the different responses and achieve the optimal extraction conditions to enhance the analytical responses of the target analytes:

$$D = (d_1(Y_1) \cdot d_2(Y_2) \cdots d_n(Y_n))^{1/n} \quad (3)$$

where n is the number of responses in the optimization process, and $d_i(Y_i)$ is the individual desirability of each response in the experiment. The individual desirability is calculated as:

$$di = Y_i - Y_{min} / Y_{max} - Y_{min} \quad (4)$$

Responses are ranked between 0 and 1, respectively, to define undesirable responses and fully desirable responses.

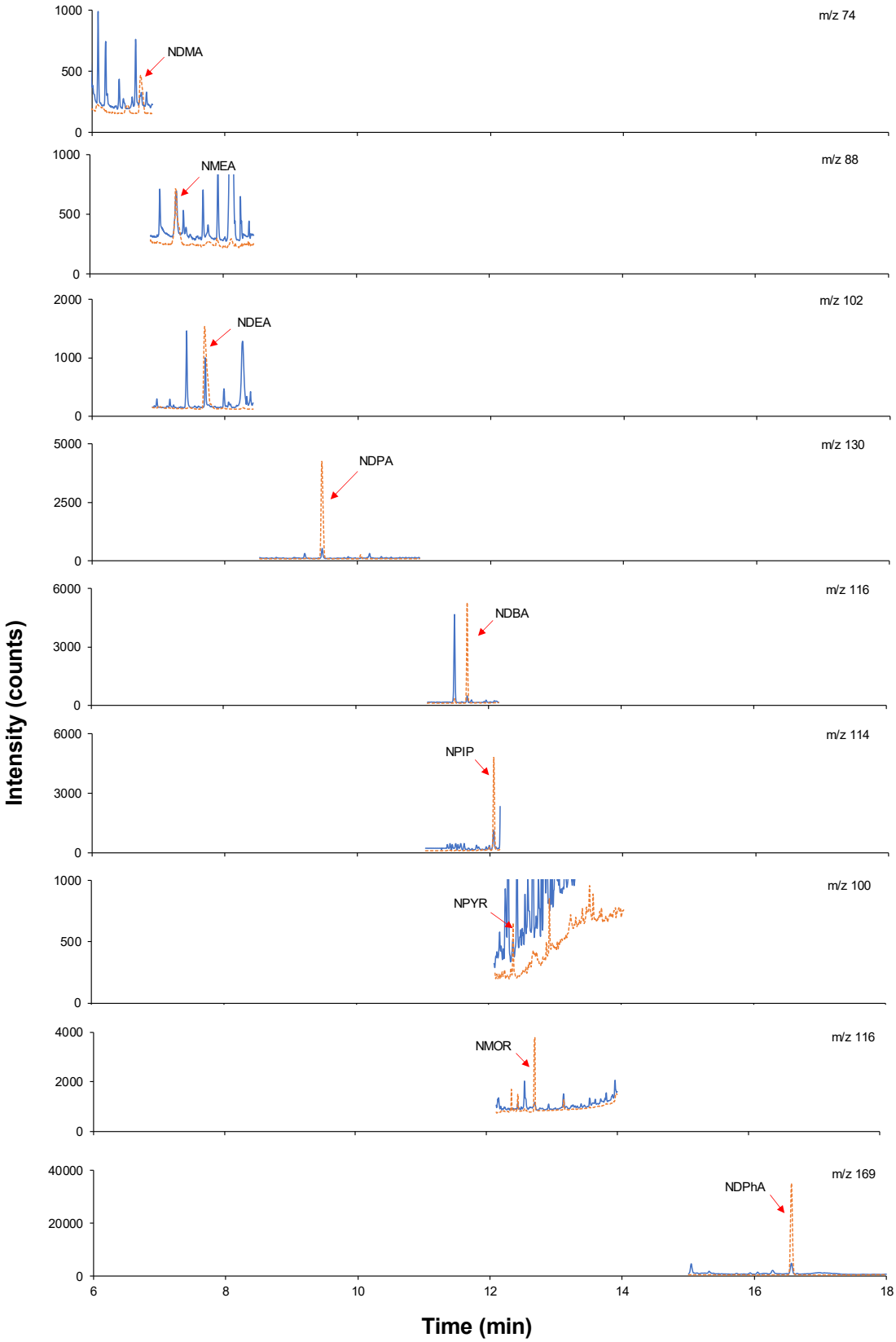

Figure S1. Chromatogram of a standard solution containing the analytes at 10 ng mL^{-1} subjected to the VA-DLLME procedure (dotted orange line), and (b) unextracted (continuous blue line).

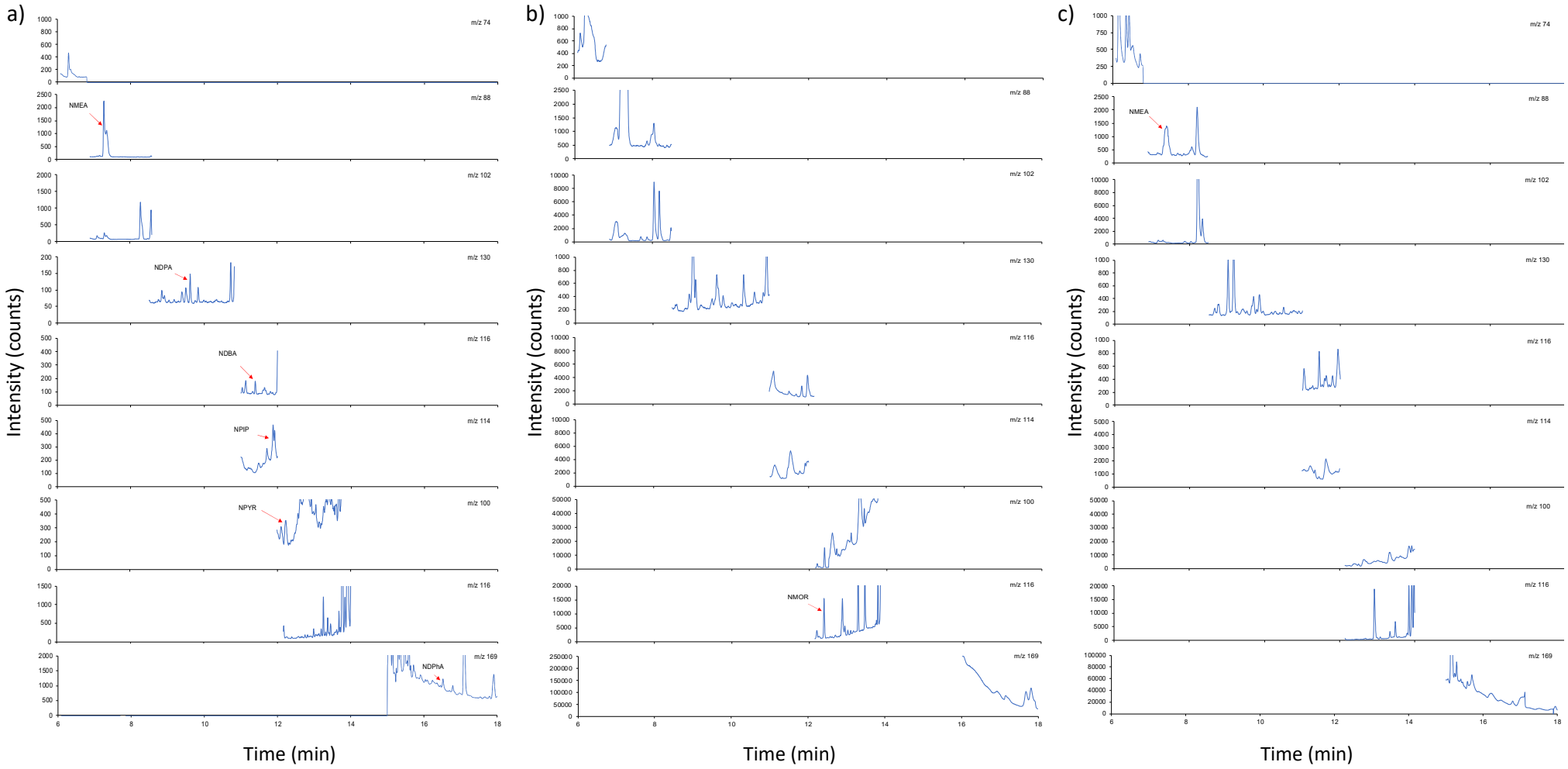

Figure S2. Chromatograms of sample solutions subjected to the proposed VA-DLLME method: (a) aftersun gel, (b) body cream 1, and (c) body cream 2.