

## Supplementary material

# Rapid Simultaneous Quantification of 1-Formyl-2,2-Dimethylhydrazine and Dimethylurea Isomers in Environmental Samples by Supercritical Fluid Chromatography - Tandem Mass Spectrometry

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## Contents

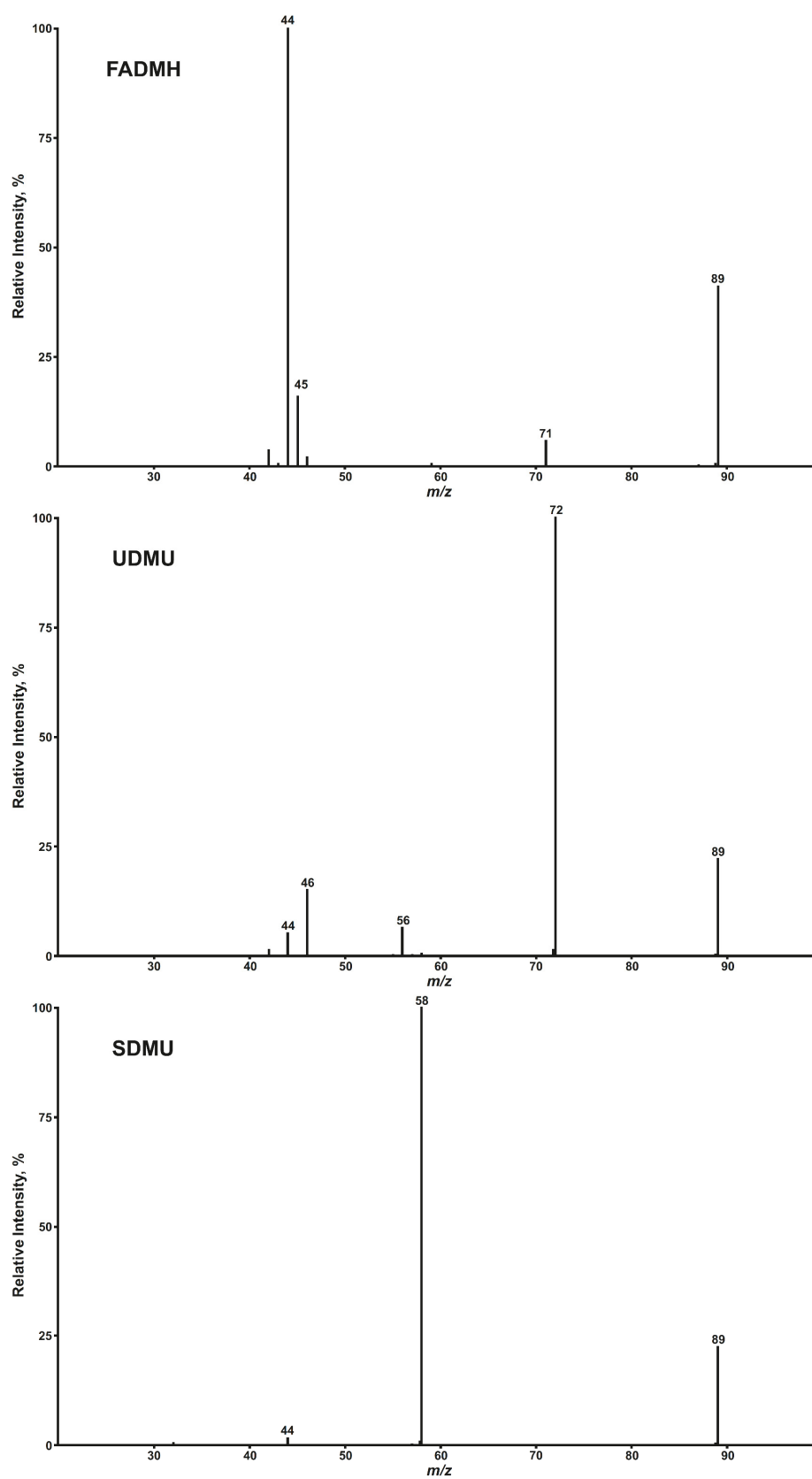
**Table S1.** Effect of SFC conditions on the parameters of chromatographic separation of analytes ( $k$  – retention factor,  $W_{1/2}$  – peak width at half-height,  $\alpha$  – selectivity,  $R$  – resolution).

**Table S2.** The intra-day and inter-day precision of the developed approach

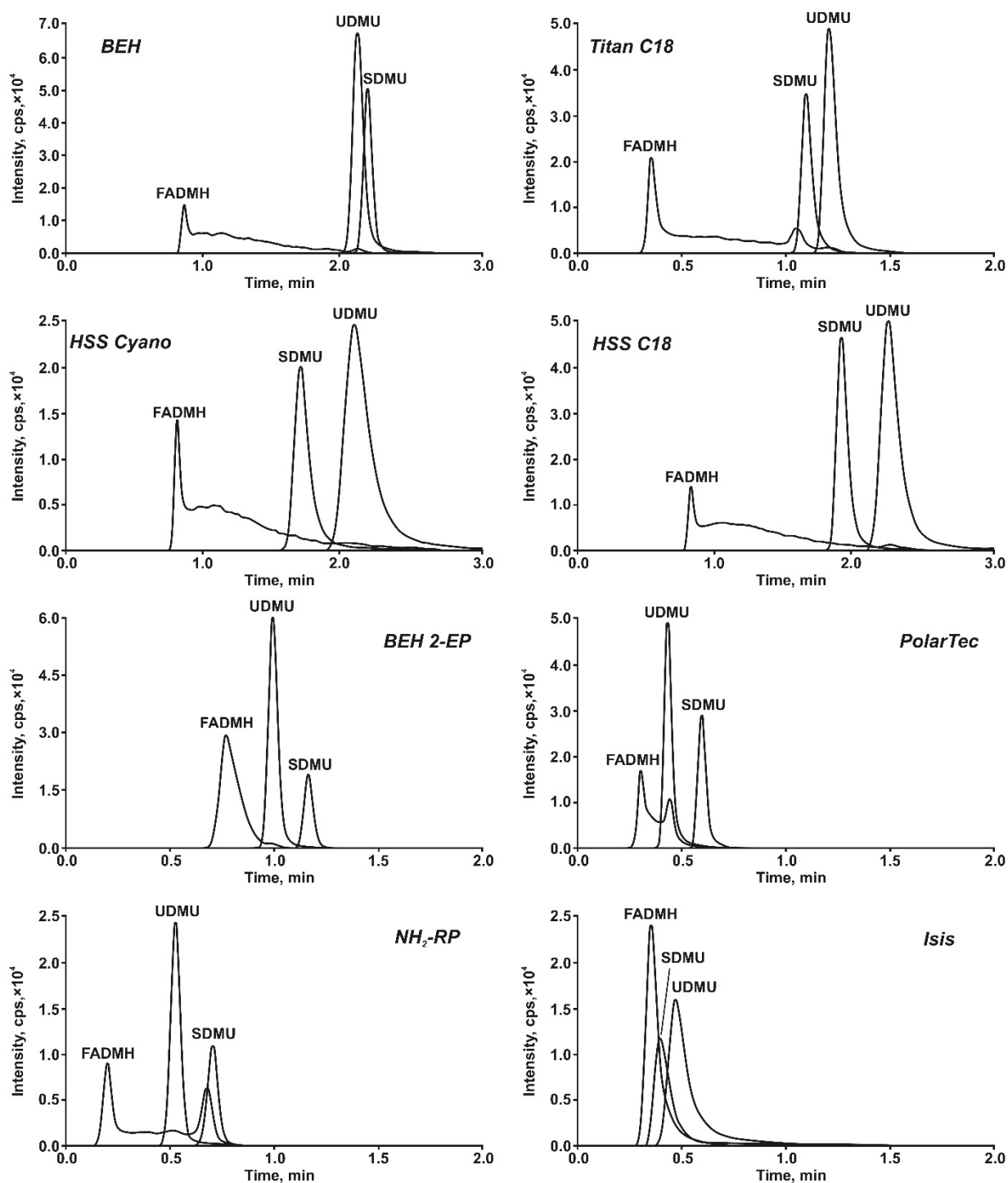
**Table S3.** In-silico predicted toxicity and mutagenicity of analytes

**Figure S1.** Tandem mass spectra of FADMH, UDMU, and SDMU. Collision energy – 30 eV with spread of 20 eV.

**Figure S2.** SFC-MS/MS chromatograms of the model mixture of analytes obtained on different stationary phases (Acquity BEH, Titan C18, Acquity HSS C18, Nucleodur ISIS, Nucleodur PolarTec, Acquity HSS Cyano, Acquity BEH 2-EP, Nucleodur NH2-RP). Analysis conditions: mobile phase – carbon dioxide with 10% of methanol, flowrate – 1.3 mL min<sup>-1</sup>, column temperature – 25°C, back pressure – 130 bar, injection volume – 2.0  $\mu$ L.



**Figure S1.** Tandem mass spectra of FADMH, UDMU, and SDMU. Collision energy – 30 eV with spread of 20 eV.



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**Table S1.** Effect of SFC conditions on the parameters of chromatographic separation of analytes (k – retention factor,  $W_{1/2}$  – peak width at half-height,  $\alpha$  – selectivity, R – resolution).

Parameter	Value	k			$W_{1/2}$			$\alpha$		R	
		FADMH	UDMU	SDMU	FADMH	UDMU	SDMU	FADMH / UDMU	UDMU / SDMU	FADMH / UDMU	UDMU / SDMU
Content of MeOH (% v/v) at 25°C and 130 bar	5	0.43	1.59	2.95	0.11	0.07	0.09	3.70	1.86	4.79	6.34
	7	0.33	1.00	1.73	0.09	0.05	0.06	3.00	1.73	3.54	4.93
	10	0.24	0.62	0.95	0.07	0.05	0.05	2.60	1.54	2.36	2.48
	12	0.19	0.48	0.70	0.06	0.05	0.05	2.50	1.47	1.93	1.65
	15	0.14	0.33	0.46	0.06	0.05	0.05	2.33	1.38	1.29	0.94
T (°C) at 10% of MeOH and 130 bar	10	0.22	0.57	0.83	0.09	0.05	0.05	2.57	1.44	1.85	1.89
	25	0.24	0.59	0.86	0.10	0.05	0.05	2.47	1.46	1.73	2.01
	40	0.24	0.59	0.89	0.09	0.05	0.05	2.47	1.51	1.85	2.24
	55	0.24	0.60	0.94	0.07	0.05	0.05	2.53	1.55	2.26	2.48
P (bar) at 10% of MeOH and 55°C	110	0.25	0.65	1.02	0.08	0.05	0.05	2.56	1.56	2.27	2.71
	130	0.24	0.60	0.95	0.07	0.05	0.05	2.53	1.58	2.26	2.60
	150	0.22	0.57	0.90	0.07	0.05	0.05	2.57	1.58	2.16	2.48
	170	0.21	0.54	0.86	0.07	0.05	0.05	2.62	1.59	2.07	2.36
	190	0.19	0.51	0.83	0.06	0.05	0.05	2.67	1.63	2.15	2.36

**Table S2.** The intra-day and inter-day precision of the developed approach

Analyte	C, $\mu\text{g L}^{-1}$	Intra-day		Inter-day	
		RSD, %	Accuracy, %	RSD, %	Accuracy, %
FADMH	12.5	14	103	14	105
	125	2	98	2	98
	3125	2	99	3	97
1,1-DMU	2.00	14	102	15	110
	20.0	2	94	4	97
	500	2	96	3	95
1,3-DMU	2.00	8	100	10	107
	20.0	3	96	3	98
	500	2	96	2	94

**Table S3.** In-silico predicted toxicity and mutagenicity of analytes

Properties	Compound		
	FADMH	UDMU	SDMU
Acute toxicity, $\text{LD}_{50}$ , $\text{mg kg}^{-1}$			
Mouse/Intraperitoneal	500	410	410
Mouse/Oral	2200	1100	1300
Rat/Intraperitoneal	500	720	420
Rat/Oral	2100	1300	1100
Aquatic toxicity, $\text{LC}_{50}$ , $\text{mg L}^{-1}$			
Pimephales promelas	280	460	19
Daphnia magna	440	750	240
Mutagenicity			
Probability of positive Ames test	0.51	0.14	0.19