

Supplemental Information

Multivariate Curve Resolution-Alternating Least Squares Analysis of High Resolution Liquid Chromatography-Mass Spectrometry Data

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Table S1. Calibration Samples for Amphetamine Analysis

	Sample ID	Concentration (ppm)																	
		PE	PPA	PEA	EP	PSE	Amp	MDA	Mamp	MDMA	Moxy	Phent	PMMA	MDE	MTA	mCPP	Bromo	Traz	BP
Blank	B1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Calibration Samples	1a	10	-	-	2	-	-	6	-	-	-	10	-	2	-	-	-	-	10
	1b	-	10	-	-	2	-	-	6	10	-	-	-	-	2	-	6	-	-
	1c	-	-	10	-	-	2	-	-	-	6	-	10	-	-	2	-	6	-
	2a	2	-	-	6	-	-	10	-	-	-	2	-	6	-	-	-	-	2
	2b	-	2	-	-	6	-	-	10	2	-	-	-	-	6	-	10	-	-
	2c	-	-	2	-	-	6	-	-	-	10	-	2	-	-	6	-	10	-
	3a	6	-	-	10	-	-	2	-	-	-	6	-	10	-	-	-	-	6
	3b	-	6	-	-	10	-	-	2	6	-	-	-	-	10	-	2	-	-
	3c	-	-	6	-	-	10	-	-	-	2	-	6	-	-	10	-	2	-
Test Mixtures	1a	4	-	-	8	-	-	4	-	-	-	8	-	4	-	-	-	-	4
	1b	-	4	-	-	8	-	-	4	8	-	-	-	-	4	-	8	-	-
	1c	-	-	4	-	-	8	-	-	-	4	-	8	-	-	4	-	8	-
	2a	8	-	-	4	-	-	8	-	-	-	4	-	8	-	-	-	-	8
	2b	-	8	-	-	4	-	-	8	4	-	-	-	-	8	-	4	-	-

Table S2. Calibration Statistics for Amphetamine Analysis.*

Statistic	PE	PPA	PEA	MDA	Phent	MDE	Mamp	MDMA	Amp	Moxy	PMMA	MTA	mCPP	Bromo	BP	Traz
Slope [10⁴] (S.D.)	18.9 (1.2)	113 (8.7)	66.5 (3.5)	152 (13)	27.9 (2.3)	72.9 (6.3)	70.6 (6.1)	61.4 (5.1)	24.9 (0.77)	45.2 (2.2)	60.3 (4.1)	51.4 (2.1)	57.4 (2.2)	29.6 (1.2)	175 (11)	109 (8.3)
Intercept [10⁴] (S.D.)	8.2 (7.3)	55 (55)	23 (22)	94 (82)	14 (14)	44 (40)	42 (39)	36 (32)	5.5 (4.8)	14 (14)	29 (26)	13 (13)	16 (14)	7.1 (7.8)	80 (67)	55 (52)
S_E [10⁴]	9.42	70.7	28.2	107	18.4	51.3	50.0	41.1	6.25	17.9	33.3	17.3	17.7	10.1	87.3	67.1
R²	0.9925	0.9882	0.9946	0.9854	0.9869	0.9852	0.9850	0.9866	0.9981	0.9952	0.9908	0.9966	0.9970	0.9965	0.9925	0.9888
ALS LOF (%)	19.8	10.2		8.95								11.0		7.47	14.7	
# Iters.	4	3		10								3		3	3	

*Statistics are shown for the final MCR-ALS analysis at the highest level of resolution.