

Supplemental Information

for

On-Site Illicit-Drug Detection with an Integrated Near-Infrared Spectral Sensor: A Proof of Concept

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Figure S1. Confusion matrices of the Set B data using 4 drug and 1 other categories.

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Set A 'common drugs-of-abuse'			Set B 'off-white casework samples'			Set C 'crushed ecstasy tablets'		
Individual analyses (N=591)	Train (N=297)	Test (N=294)	Individual samples (N=246)	Train (N=193)	Test (N=53)	Individual samples (N=71)	Train (N=52)	Test (N=19)
MDMA	27	26	cocaine	125	30	MDMA	28	11
amphetamine	27	27	ketamine	12	6	others	24	8
caffeine	27	27	amphetamine	12	6			
cocaine HCl	27	27	MDMA	7	6			
cocaine base	27	27	others	37	5			
heroin	27	25						
ketamine	27	27						
levamisole	27	26						
lidocaine	27	27						
methamphetamine	27	27						
paracetamol	27	27						

Table S1. Composition of the test and training sets for all sample sets. For set A the numbers depict replicate measurements (3-scan average) of the same sample. For sets B and C the values depict individual samples. For each sample 9 underlying measurements were included.

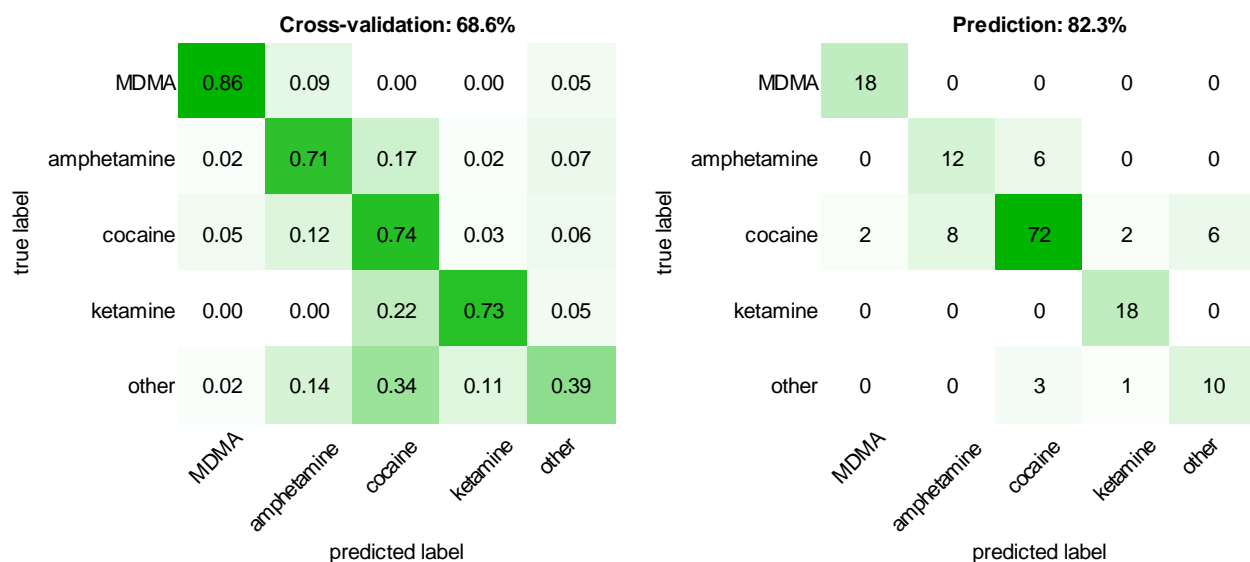


Figure S1. Confusion matrices of the Set B data using 4 drug and 1 other categories. Results following SNV pre-processing and LDA classification.

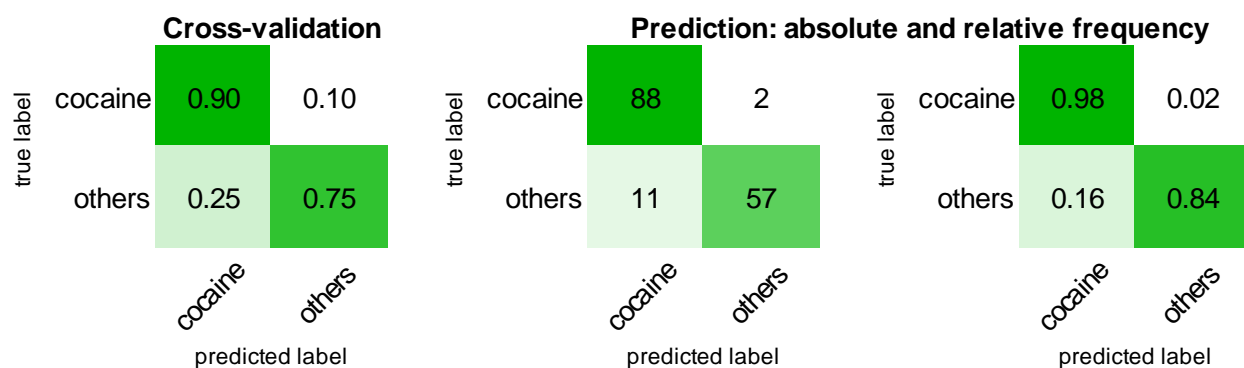


Figure S2. Confusion matrices of the Set B data processed as a cocaine detection test. Results following SNV pre-processing and PLS-RF classification.