

Supplemental Information

for

On-site forensic analysis of colored seized materials: detection of brown heroin and MDMA-tablets by a portable NIR spectrometer

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Table S1. Performance of the chemometric model on the various sample sets, results in samples.

Individual results for all scans and samples can be found in the following separate supplementary files:

- Results per sample_heroin matrix.pdf**
Results per sample_MDMA matrix both forms.pdf
Results per sample_MDMA matrix hydrate only.pdf

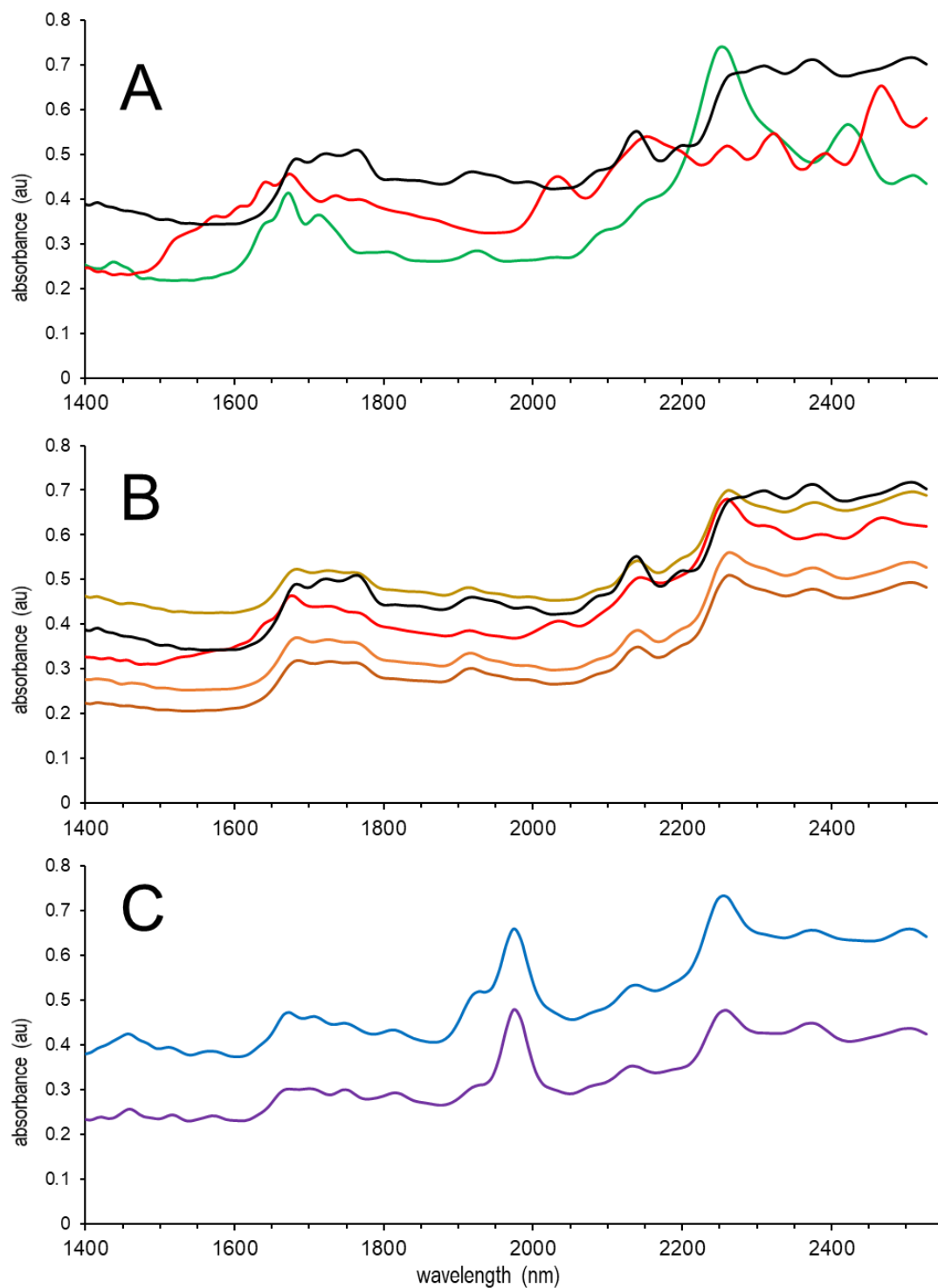


Figure S1. NIR spectra (raw) of heroin base (black trace in panels A and B) compared to common adulterants (panel A) and various brown heroin casework samples (panel B). Panel A: paracetamol (red), caffeine (green). Panel B: brown heroin samples (brown to orange shades), brown heroin sample highly adulterated with paracetamol and caffeine, H19 (red). Panel C depicts heroin HCl·H₂O (purple) and a white heroin casework sample, H8 (blue).

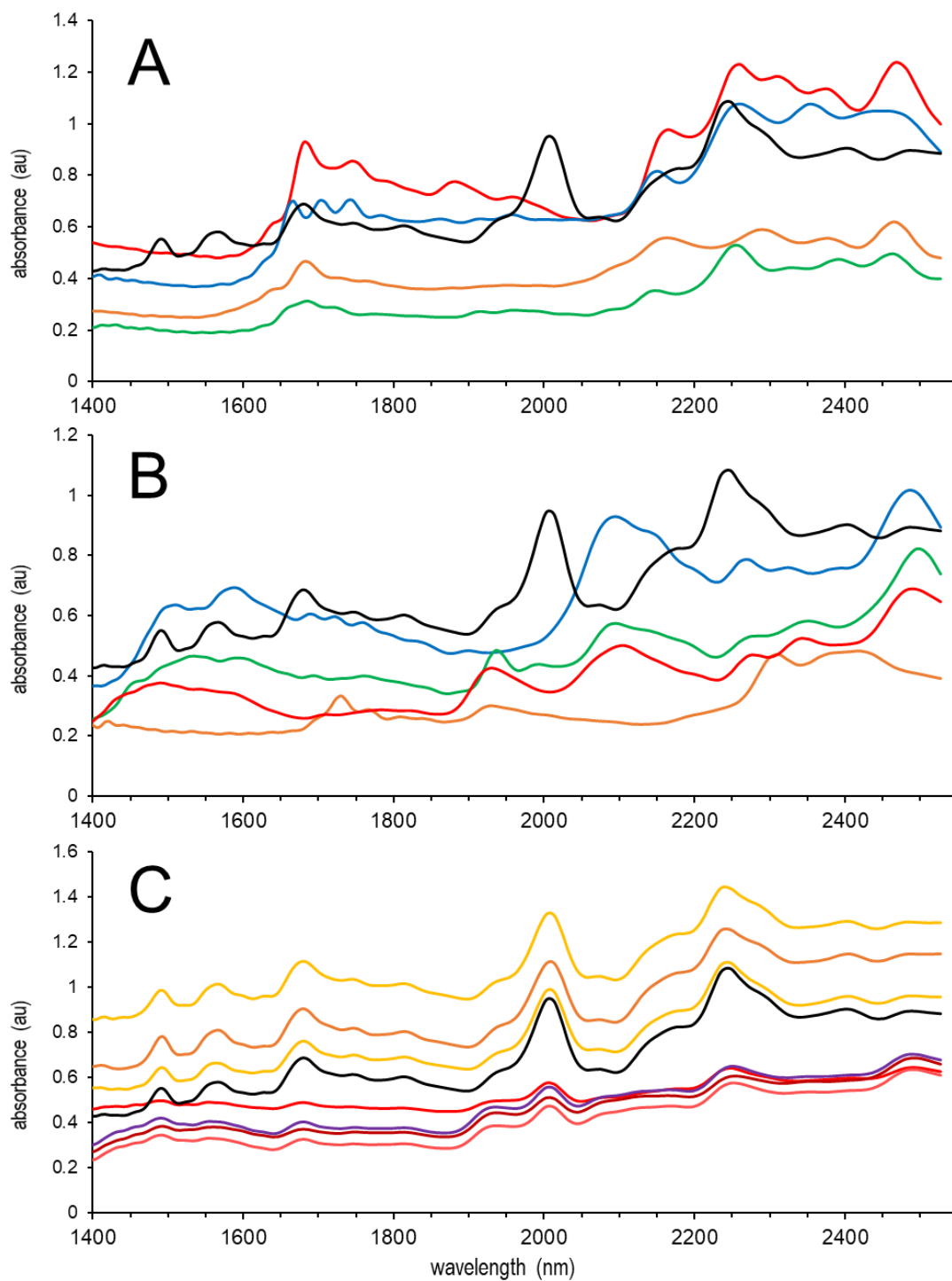


Figure S2. NIR spectra (raw) of MDMA HCl (black trace in all panels) compared to other drugs (panel A), common excipients (panel B) and various MDMA-containing casework samples (panel C). Panel A: methamphetamine HCl (red), cocaine HCl (green), ketamine (blue), amphetamine sulphate (orange). Panel B: microcrystalline cellulose (red), lactose (green), mannitol (blue), Mg stearate (orange). Panel C: MDMA crystals, M1-3 (orange shades), crushed MDMA-containing ecstasy tablets, P1-4 (purple to red shades).

Table S1. Performance of the chemometric model on the various sample sets, results in samples

heroin matrix library						
sample set	pos#	TP	FN	neg#	TN	FP
H	46	42	4*	9	9	0
M	0	0	0	11	11	0
P	0	0	0	71	71	0
T	0	0	0	71	71	0
T2	0	0	0	65	65	0
C,D,N	3	3	0	92	92	0
PAM	0	0	0	181	181	0
TOTAL	49	45	4	500	500	0
MDMA matrix library (incl. anhydride)						
sample set	pos#	TP	FN	neg#	TN	FP
H	0	0	0	55	55	0
M	11	11	0	0	0	0
P	39	37	2**	32	32	0
T	39	37	2	32	32	0
T2	47	44	3	18	18	0
C,D,N	3	3	0	92	91	1
PAM	13	13	0	168	167	1
TOTAL	152	145	7	397	395	2
MDMA matrix library (excl. anhydride)						
sample set	pos#	TP	FN	neg#	TN	FP
H	0	0	0	55	54	1
M	11	11	0	0	0	0
P	39	37	2**	32	32	0
T	39	37	2	32	32	0
T2	47	44	3	18	18	0
C,D,N	3	3	0	92	92	0
PAM	13	13	0	168	168	0
TOTAL	152	145	7	397	396	1

Results per sample were calculated by majority voting of the individual scans. * For 3 samples in set H, 7 out of the 9 scans resulted in a match score between 0.70 - 0.80 (below threshold) for heroin. ** For one sample in set P, two out of the three scans resulted in a match score between 0.70 - 0.80 (below threshold) for MDMA. These samples were considered false negatives in this study.