

Supplemental Information

for

The influence of water of crystallization in NIR-based MDMA HCl detection

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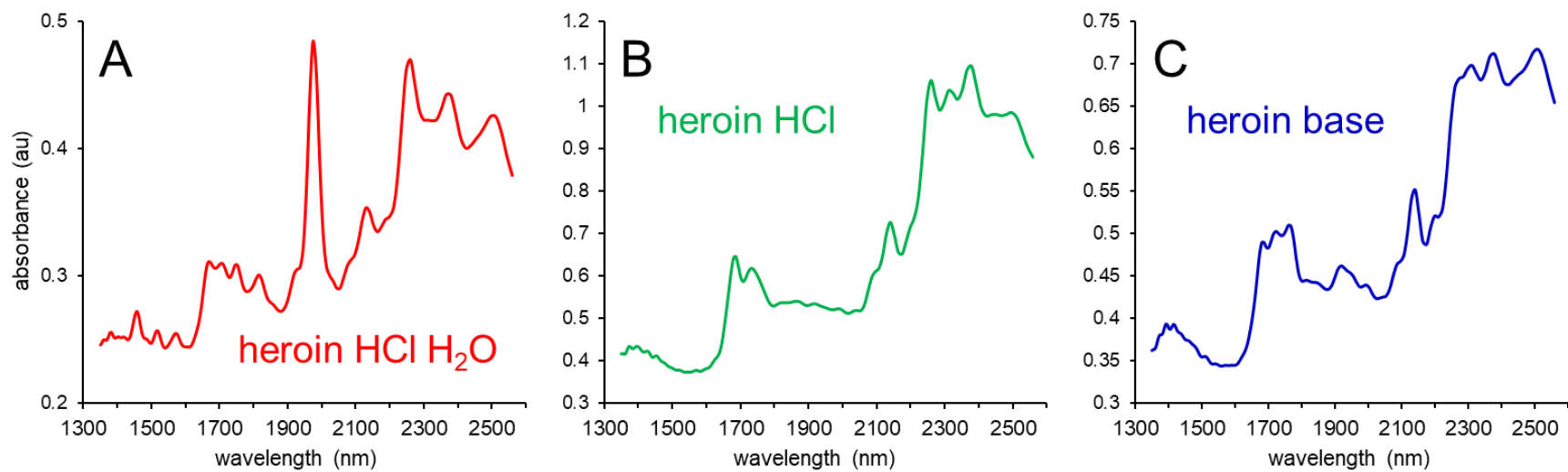


Figure S1. NIR-spectra of the various forms of heroin: heroin HCl hydrate (panel A, red), anhydrous heroin HCl (panel B, green), and the freebase form of heroin (panel C, blue).

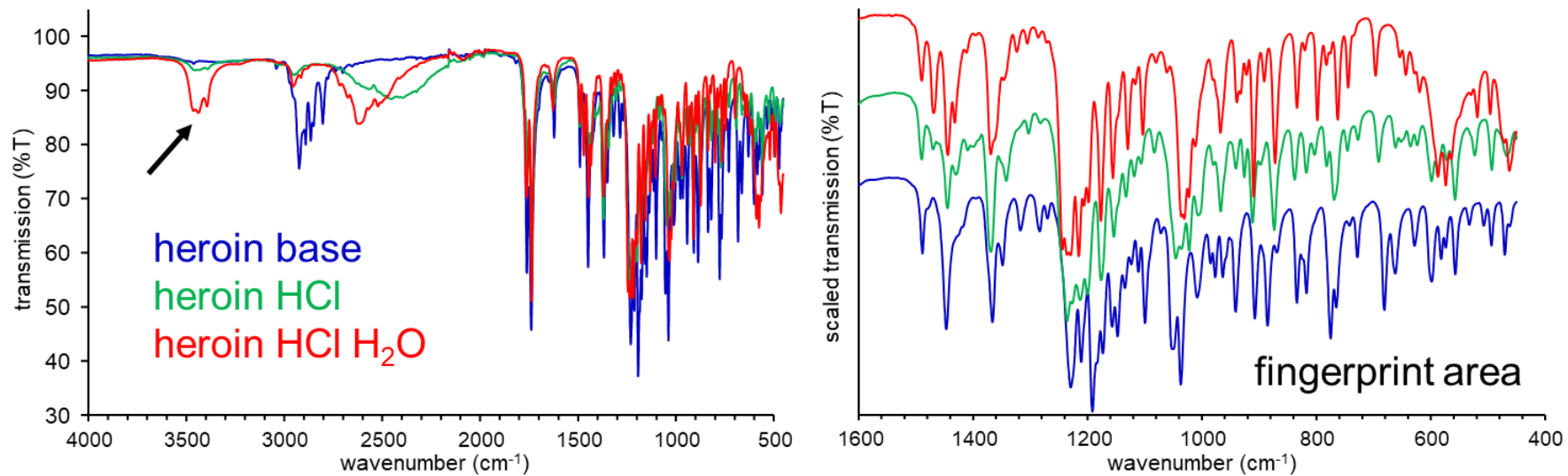


Figure S2. ATR-FTIR spectra of the heroin variants: hydrated heroin HCl (red plot); anhydrous heroin HCl (green plot); heroin base (blue plot). The arrow depicts the 3400 cm⁻¹ peak attributed to water of crystallization.

Table S1. Identification results of the drying experiments on MDMA HCl, individual results

Sample	Model result	Similarity
MDMA HCl, no treatment	MDMA HCl hydrate (99%)	0.99
MDMA HCl, no treatment	MDMA HCl hydrate (99%)	0.99
MDMA HCl, no treatment	MDMA HCl hydrate (99%)	0.99
MDMA HCl, dried 1 min @ 100 °C	MDMA HCl hydrate (31%) + MDMA HCl (anhydrous) (66%)	0.97
MDMA HCl, dried 1 min @ 100 °C	MDMA HCl hydrate (27%) + MDMA HCl (anhydrous) (70%)	0.97
MDMA HCl, dried 1 min @ 100 °C	MDMA HCl hydrate (29%) + MDMA HCl (anhydrous) (69%)	0.98
MDMA HCl, dried 2 min @ 100 °C	MDMA HCl hydrate (19%) + MDMA HCl (anhydrous) (75%)	0.94
MDMA HCl, dried 2 min @ 100 °C	MDMA HCl hydrate (27%) + MDMA HCl (anhydrous) (68%)	0.95
MDMA HCl, dried 2 min @ 100 °C	MDMA HCl hydrate (32%) + MDMA HCl (anhydrous) (65%)	0.98
MDMA HCl, dried 3 min @ 100 °C	MDMA HCl hydrate (19%) + MDMA HCl (anhydrous) (75%)	0.94
MDMA HCl, dried 3 min @ 100 °C	MDMA HCl hydrate (16%) + MDMA HCl (anhydrous) (78%)	0.94
MDMA HCl, dried 3 min @ 100 °C	MDMA HCl hydrate (16%) + MDMA HCl (anhydrous) (79%)	0.95
MDMA HCl, dried 4 min @ 100 °C	MDMA HCl (anhydrous) (71%)	0.91
MDMA HCl, dried 4 min @ 100 °C	MDMA HCl (anhydrous) (72%)	0.92
MDMA HCl, dried 4 min @ 100 °C	MDMA HCl (anhydrous) (77%)	0.93
MDMA HCl, dried 5 min @ 100 °C	MDMA HCl (anhydrous) (69%)	0.90
MDMA HCl, dried 5 min @ 100 °C	MDMA HCl (anhydrous) (73%)	0.91
MDMA HCl, dried 5 min @ 100 °C	MDMA HCl (anhydrous) (71%)	0.92
MDMA HCl, dried 6 min @ 100 °C	MDMA HCl (anhydrous) (73%)	0.93
MDMA HCl, dried 6 min @ 100 °C	MDMA HCl (anhydrous) (75%)	0.93
MDMA HCl, dried 6 min @ 100 °C	MDMA HCl (anhydrous) (71%)	0.92
MDMA HCl, dried 7 min @ 100 °C	MDMA HCl (anhydrous) (79%)	0.94
MDMA HCl, dried 7 min @ 100 °C	MDMA HCl (anhydrous) (81%)	0.94
MDMA HCl, dried 7 min @ 100 °C	MDMA HCl (anhydrous) (78%)	0.94
MDMA HCl, dried 8 min @ 100 °C	MDMA HCl (anhydrous) (78%)	0.94
MDMA HCl, dried 8 min @ 100 °C	MDMA HCl (anhydrous) (78%)	0.94
MDMA HCl, dried 8 min @ 100 °C	MDMA HCl (anhydrous) (78%)	0.94
MDMA HCl, dried 9 min @ 100 °C	MDMA HCl (anhydrous) (81%)	0.95
MDMA HCl, dried 9 min @ 100 °C	MDMA HCl (anhydrous) (94%)	0.94
MDMA HCl, dried 9 min @ 100 °C	MDMA HCl (anhydrous) (80%)	0.94
MDMA HCl, dried 10 min @ 100 °C	MDMA HCl (anhydrous) (96%)	0.96
MDMA HCl, dried 10 min @ 100 °C	MDMA HCl (anhydrous) (95%)	0.95
MDMA HCl, dried 10 min @ 100 °C	MDMA HCl (anhydrous) (94%)	0.94
MDMA HCl, dried 15 min @ 100 °C	MDMA HCl (anhydrous) (95%)	0.95
MDMA HCl, dried 15 min @ 100 °C	MDMA HCl (anhydrous) (95%)	0.95
MDMA HCl, dried 15 min @ 100 °C	MDMA HCl (anhydrous) (81%)	0.95
MDMA HCl, dried 20 min @ 100 °C	MDMA HCl (anhydrous) (95%)	0.95
MDMA HCl, dried 20 min @ 100 °C	MDMA HCl (anhydrous) (96%)	0.96
MDMA HCl, dried 20 min @ 100 °C	MDMA HCl (anhydrous) (96%)	0.96

Table S2. Identification results of the recovery experiments at ambient conditions on anhydrous MDMA HCl, individual results

Sample	Model result	Similarity
MDMA HCl, dried 3 hr @ 100 °C	MDMA HCl (anhydrous) (99%)	0.99
MDMA HCl, dried 3 hr @ 100 °C	MDMA HCl (anhydrous) (99%)	0.99
MDMA HCl, dried 3 hr @ 100 °C	MDMA HCl (anhydrous) (98%)	0.98
MDMA HCl, after 6 days	MDMA HCl (anhydrous) (98%)	0.98
MDMA HCl, after 6 days	MDMA HCl (anhydrous) (98%)	0.98
MDMA HCl, after 6 days	MDMA HCl (anhydrous) (98%)	0.98
MDMA HCl, after 12 days	MDMA HCl hydrate (15%) + MDMA HCl (anhydrous) (84%)	0.98
MDMA HCl, after 12 days	MDMA HCl hydrate (15%) + MDMA HCl (anhydrous) (84%)	0.98
MDMA HCl, after 12 days	MDMA HCl hydrate (14%) + MDMA HCl (anhydrous) (84%)	0.98
MDMA HCl, after 19 days	MDMA HCl hydrate (45%) + MDMA HCl (anhydrous) (52%)	0.97
MDMA HCl, after 19 days	MDMA HCl hydrate (43%) + MDMA HCl (anhydrous) (55%)	0.99
MDMA HCl, after 19 days	MDMA HCl hydrate (40%) + MDMA HCl (anhydrous) (58%)	0.98
MDMA HCl, after 27 days	MDMA HCl hydrate (35%) + MDMA HCl (anhydrous) (62%)	0.97
MDMA HCl, after 27 days	MDMA HCl hydrate (33%) + MDMA HCl (anhydrous) (64%)	0.97
MDMA HCl, after 27 days	MDMA HCl hydrate (32%) + MDMA HCl (anhydrous) (66%)	0.98
MDMA HCl, after 47 days	MDMA HCl hydrate (32%) + MDMA HCl (anhydrous) (66%)	0.98
MDMA HCl, after 47 days	MDMA HCl hydrate (35%) + MDMA HCl (anhydrous) (62%)	0.97
MDMA HCl, after 47 days	MDMA HCl hydrate (31%) + MDMA HCl (anhydrous) (67%)	0.98
MDMA HCl, after 61 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 61 days	MDMA HCl hydrate (98%)	0.98
MDMA HCl, after 61 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 76 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 76 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 76 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 82 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 82 days	MDMA HCl hydrate (99%)	0.99
MDMA HCl, after 82 days	MDMA HCl hydrate (99%)	0.99

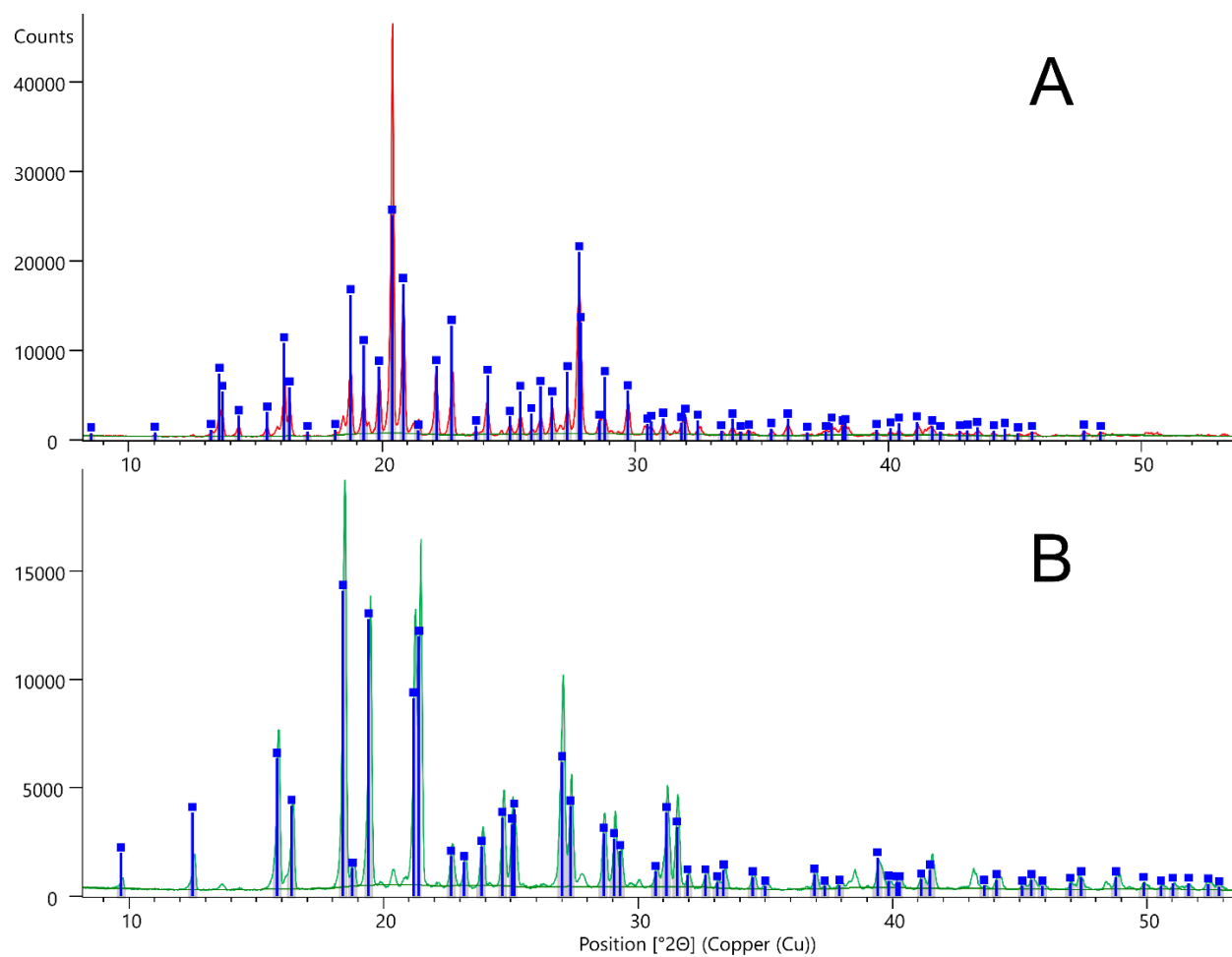


Figure S3. XRD diffraction pattern of hydrated (A) and anhydrous (B) MDMA HCl in overlay with their ICDD database matches: measured MDMA HCl hydrate (red line), anhydrous MDMA HCl obtained after drying (green line) and corresponding library match spectra with ‘ecstasy hydrate 00-065-0858’ (blue bars in panel A) and ‘ecstasy 00-064-1315’ (blue bars in panel B). Both matches were the best obtained matches from the automated search in the ICDD library with candidate match scores of 73 for ecstasy hydrate and 58 for ecstasy. The matches were confirmed after manual inspection by the XRD expert.

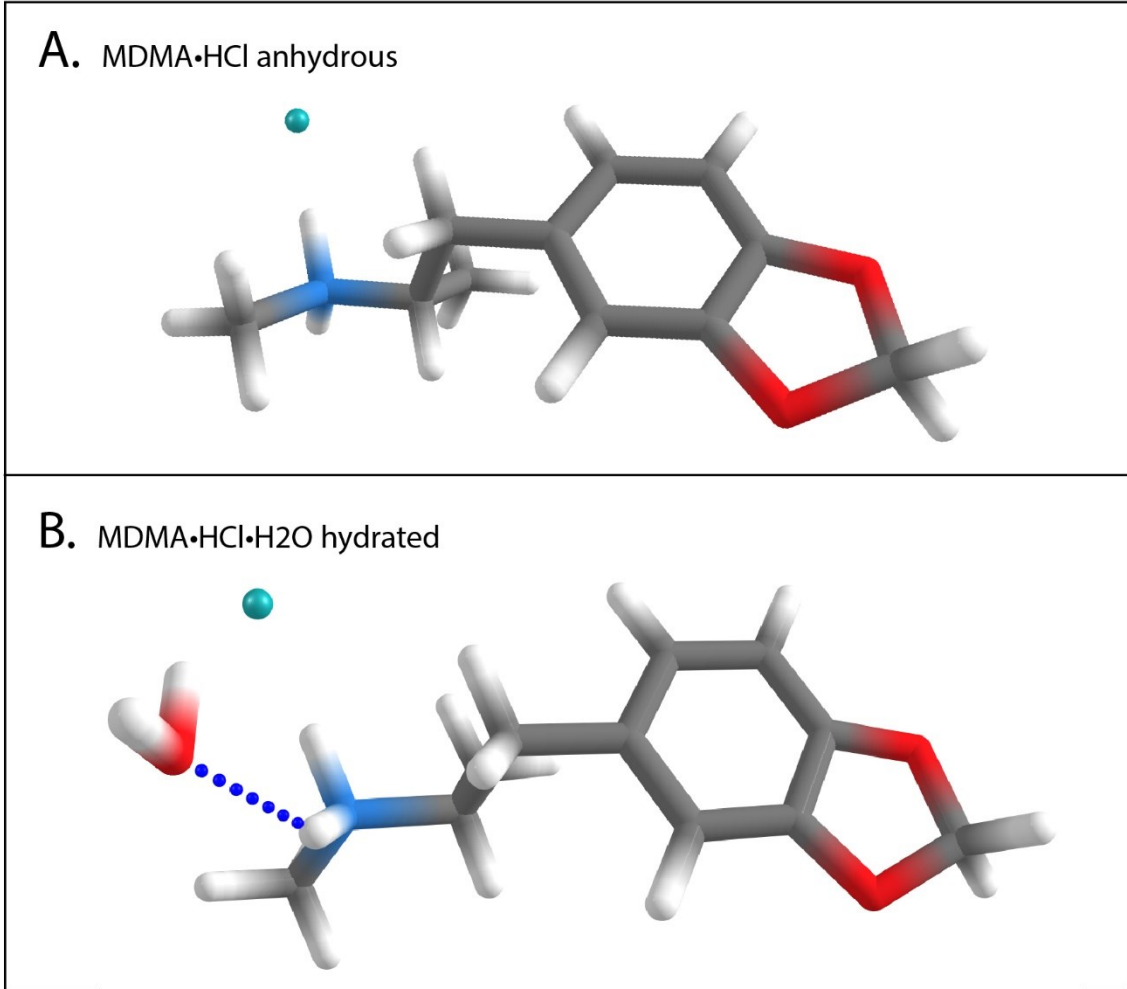


Figure S4. Molecular structures used for the DFT calculation leading to the calculated spectra shown in Figure 5. Anhydrous MDMA·HCl (A) and hydrated MDMA·HCl·H₂O (B).