

# Supplemental Information

for

## Portable near-infrared detection to replace color tests in an analytical scheme for forensic drug identification

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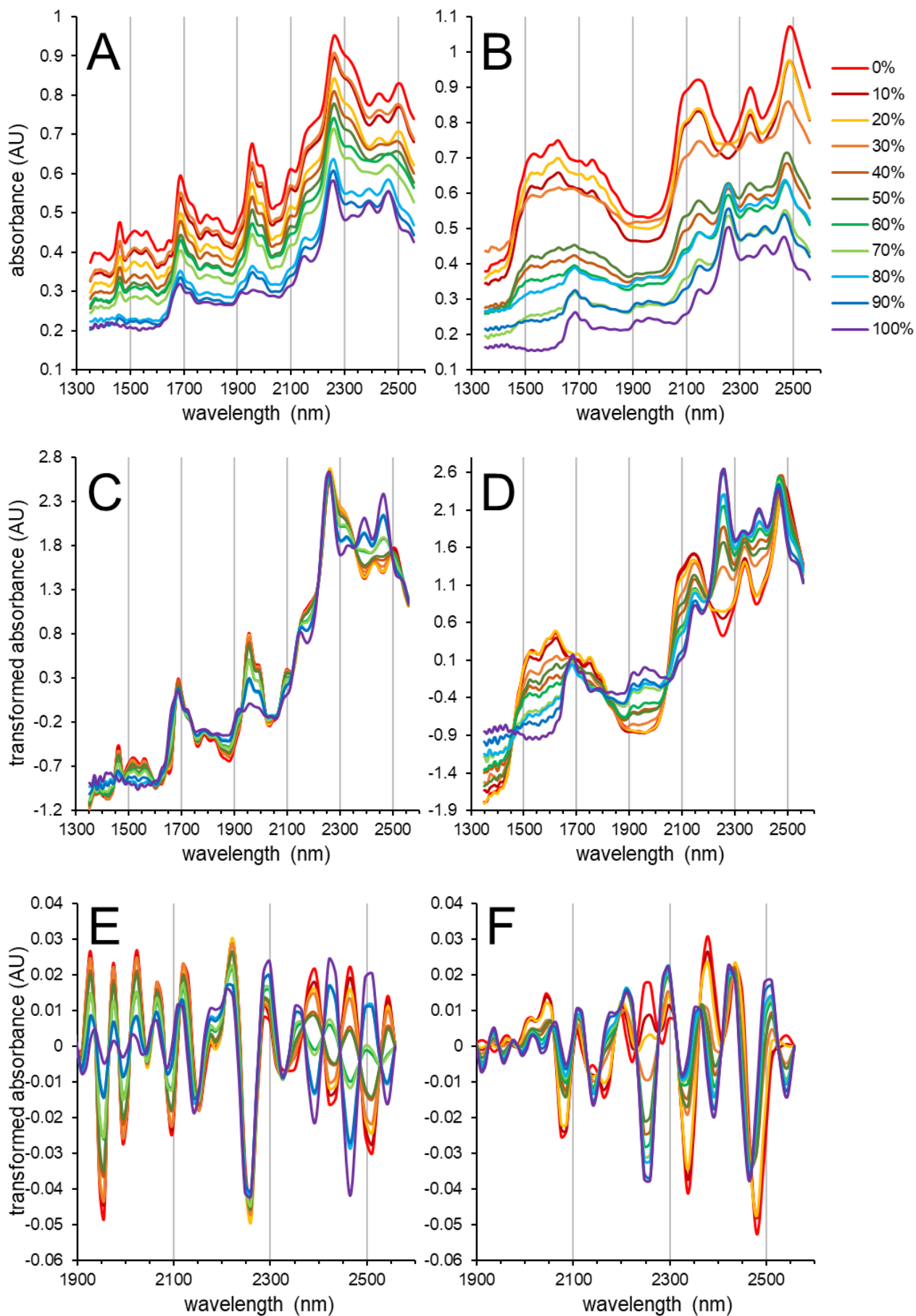
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**Figure S1.** NIR-spectra of binary cocaine mixtures with lidocaine and inositol. Raw data, SNV, and 2<sup>nd</sup> derivatives.

**Table S1.** Comparison of GC-MS and NIR results for 516 casework samples



**Figure S1.** NIR-spectra of 0 – 100% cocaine HCl mixtures with lidocaine (left column, A,C,E) and inositol (right column, B,D,F). Panels A+B: raw NIR diffuse reflectance data. Panels C+D: Standard normal variate (SNV) normalized data of panels A+B. Panels E+F: Second derivative spectra of panel A+B data.

**Table S1. (part 1 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050514	amphetamine	Inconclusive	
B050515	amphetamine	amphetamine sulphate	
B050521	amphetamine	amphetamine sulphate + Caffeine	
B050528	amphetamine	amphetamine sulphate + Caffeine	
B050769	amphetamine	amphetamine sulphate + Caffeine	
B050789	amphetamine	amphetamine sulphate	
B050862	amphetamine	amphetamine sulphate + Caffeine	
B050876	amphetamine	Inositol (45%)	
B050878	amphetamine	amphetamine sulphate	
B051139	amphetamine	Inconclusive	beige powder
B051169	amphetamine	amphetamine sulphate + Caffeine	
B051270	amphetamine	amphetamine sulphate + Caffeine	
B051395	amphetamine	amphetamine sulphate + Caffeine	
B051400	amphetamine	amphetamine sulphate	
B051503	amphetamine	amphetamine sulphate	
B051550	amphetamine	amphetamine sulphate + Caffeine	
B051574	amphetamine	amphetamine sulphate	
B051583	amphetamine	amphetamine sulphate	
B050142	CMC	Inconclusive	
B050144	CMC	Inconclusive	
B050220	CMC	Inconclusive	
B050439	CMC	Inconclusive	
B050443	CMC	Inconclusive	
B050444	CMC	Inconclusive	
B050445	CMC	Inconclusive	
B050480	CMC	Inconclusive	
B050482	CMC	Inconclusive	
B050516	CMC	Cocaine HCl (24%)	
B050518	CMC	Cocaine HCl (24%)	
B050544	CMC	Inconclusive	
B050598	CMC	Inconclusive	
B050599	CMC	Cocaine HCl (30%)	
B050755	CMC	Inconclusive	
B050756	CMC	Inconclusive	
B050757	CMC	Inconclusive	
B050758	CMC	Inconclusive	
B050844	CMC	Inconclusive	
B050846	CMC	Inconclusive	
B050853	CMC	Inconclusive	
B050858	CMC	Inconclusive	
B050860	CMC	Inconclusive	
B051045	CMC	3-FMA + 4-MMC + 4-FMA	
B051141	CMC	3-FMA + 4-MMC	
B051143	CMC	4-FMA + 4-MMC	
B051146	CMC	Inconclusive	
B051150	CMC	Inconclusive	
B051151	CMC	Inconclusive	
B051257	CMC	Inconclusive	
B051272	CMC	Inconclusive	
B051273	CMC	3-FMA + 3MMC	
B051278	CMC	Ketamine + Methamphetamine	
B051494	CMC	Inconclusive	
B051495	CMC	Inconclusive	
B051519	CMC	Inconclusive	
B051521	CMC	Inconclusive	
B051538	CMC	Inconclusive	
B050446	CMC	Inconclusive	

Legend:

- correct result (true positive or true negative)
- false negative
- substance not in NIR library
- incorrect (not all drugs correct, wrong drug detected)

**Table S1. (part 2 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050130	Cocaine	Cocaine HCl + Inositol	
B050151	Cocaine	Cocaine HCl	
B050152	Cocaine	Cocaine HCl	
B050153	Cocaine	Cocaine HCl	
B050154	Cocaine	Cocaine HCl	
B050155	Cocaine	Cocaine HCl	
B050156	Cocaine	Cocaine HCl + Levamisole HCl	
B050157	Cocaine	Cocaine Base	
B050158	Cocaine	Cocaine base + Phenacetin	
B050160	Cocaine	Cocaine base + Phenacetin	
B050163	Cocaine	Cocaine HCl	
B050165	Cocaine	Cocaine HCl	
B050167	Cocaine	Cocaine HCl	
B050169	Cocaine	Cocaine base	
B050198	Cocaine	Cocaine base	
B050200	Cocaine	Cocaine HCl	
B050226	Cocaine	Cocaine base + Inositol	
B050227	Cocaine	Cocaine base + Inositol	
B050228	Cocaine	Cocaine HCl	
B050229	Cocaine	Cocaine HCl	
B050232	Cocaine	Cocaine HCl	
B050233	Cocaine	Cocaine HCl	
B050234	Cocaine	Cocaine HCl	
B050235	Cocaine	Cocaine HCl	
B050237	Cocaine	Cocaine base	
B050238	Cocaine	Cocaine base	
B050240	Cocaine	Cocaine base	
B050241	Cocaine	Cocaine base	
B050243	Cocaine	Cocaine base	
B050245	Cocaine	Cocaine HCl + Inositol	
B050247	Cocaine	Cocaine HCl	
B050248	Cocaine	Cocaine base + Levamisol	
B050249	Cocaine	Cocaine HCl	
B050250	Cocaine	Cocaine base	
B050302	Cocaine	Cocaine base	
B050308	Cocaine	Cocaine HCl + Inositol	
B050309	Cocaine	Procaine HCl + Inositol + Cocaine base	
B050310	Cocaine	Cocaine base + Phenacetin	
B050314	Cocaine	Cocaine HCl + Mannitol	
B050321	Cocaine	Cocaine base + Phenacetin	
B050323	Cocaine	Cocaine HCl + Phenacetin	
B050324	Cocaine	Cocaine HCl + Phenacetin	
B050325	Cocaine	Cocaine HCl + Phenacetin	
B050326	Cocaine	Cocaine HCl (35%)	
B050327	Cocaine	Cocaine HCl + Phenacetin	
B050328	Cocaine	Cocaine HCl + Phenacetin	
B050329	Cocaine	Cocaine HCl + Phenacetin	
B050330	Cocaine	Cocaine HCl + Phenacetin	
B050331	Cocaine	Cocaine HCl + Phenacetin	
B050332	Cocaine	Cocaine HCl + Phenacetin	
B050333	Cocaine	Cocaine HCl + Phenacetin	
B050335	Cocaine	Cocaine HCl + Phenacetin	
B050336	Cocaine	Cocaine HCl	
B050338	Cocaine	Cocaine HCl	
B050339	Cocaine	Cocaine HCl	
B050409	Cocaine	Cocaine HCl	
B050411	Cocaine	Cocaine base	
B050415	Cocaine	Cocaine HCl + Inositol	
B050416	Cocaine	Cocaine HCl	

**Table S1. (part 3 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050422	Cocaine	Cocaine base	
B050423	Cocaine	Cocaine HCl	
B050424	Cocaine	Cocaine HCl	
B050426	Cocaine	Cocaine base	
B050428	Cocaine	Cocaine HCl + Inositol	
B050429	Cocaine	Cocaine HCl	
B050469	Cocaine	Cocaine HCl	
B050478	Cocaine	Cocaine HCl + Inositol	
B050492	Cocaine	Cocaine base + Inositol	
B050493	Cocaine	Cocaine base + Phenacetin	
B050494	Cocaine	Cocaine HCl + Phenacetin	
B050523	Cocaine	Cocaine base	
B050538	Cocaine	Cocaine HCl + Inositol	
B050539	Cocaine	Cocaine HCl	
B050540	Cocaine	Cocaine HCl	
B050542	Cocaine	Cocaine HCl	
B050545	Cocaine	Cocaine base	
B050565	Cocaine	Cocaine HCl	
B050566	Cocaine	Cocaine HCl	
B050571	Cocaine	Cocaine HCl + Inositol	
B050595	Cocaine	Cocaine HCl	
B050596	Cocaine	Cocaine HCl	
B050600	Cocaine	Cocaine base	
B050601	Cocaine	Cocaine base	
B050604	Cocaine	Cocaine base	
B050605	Cocaine	Cocaine base + Levamisol HCl	
B050606	Cocaine	Cocaine base	
B050690	Cocaine	Cocaine HCl	
B050718	Cocaine	Cocaine base	
B050733	Cocaine	Cocaine base	
B050734	Cocaine	Cocaine base + Phenacetin	
B050735	Cocaine	Cocaine base	
B050738	Cocaine	Cocaine HCl	
B050739	Cocaine	Cocaine HCl	
B050773	Cocaine	Cocaine HCl	
B050774	Cocaine	Cocaine HCl + Inositol	
B050778	Cocaine	Cocaine HCl + Inositol	
B050779	Cocaine	Cocaine HCl	
B050790	Cocaine	Cocaine HCl + Inositol	
B050796	Cocaine	Cocaine HCl	
B050827	Cocaine	Cocaine base	
B050828	Cocaine	Cocaine HCl	
B050829	Cocaine	Cocaine HCl	
B050830	Cocaine	Cocaine HCl	
B050831	Cocaine	Cocaine HCl	
B050833	Cocaine	Cocaine HCl	
B050834	Cocaine	Cocaine HCl	
B050835	Cocaine	Cocaine base	
B050837	Cocaine	Cocaine HCl	
B050850	Cocaine	Cocaine HCl	
B050851	Cocaine	Cocaine HCl	
B050852	Cocaine	Cocaine HCl	
B050854	Cocaine	Cocaine base	
B050857	Cocaine	Cocaine base	
B050868	Cocaine	Cocaine HCl	
B050869	Cocaine	Cocaine HCl	
B050870	Cocaine	Cocaine HCl	
B050871	Cocaine	Cocaine HCl	
B050872	Cocaine	Cocaine HCl	

**Table S1. (part 4 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050873	Cocaine	Cocaine HCl	
B050877	Cocaine	Cocaine HCl + Levamisole HCl	
B050880	Cocaine	Cocaine HCl + Inositol	
B050881	Cocaine	Cocaine HCl + Mannitol	
B050884	Cocaine	Cocaine HCl	
B050885	Cocaine	Cocaine HCl	
B050886	Cocaine	Cocaine HCl	
B050887	Cocaine	Cocaine HCl	
B050888	Cocaine	Cocaine HCl	
B050889	Cocaine	Cocaine HCl + Inositol	
B050890	Cocaine	Cocaine HCl	
B050891	Cocaine	Cocaine HCl	
B050892	Cocaine	Cocaine HCl	
B050894	Cocaine	Cocaine HCl + Inositol	
B050897	Cocaine	Cocaine HCl	
B050899	Cocaine	Cocaine base	
B051033	Cocaine	Cocaine HCl	
B051037	Cocaine	Cocaine HCl + Inositol	
B051039	Cocaine	Cocaine HCl	
B051067	Cocaine	Cocaine base	
B051080	Cocaine	Cocaine HCl	
B051082	Cocaine	Cocaine base	
B051084	Cocaine	Cocaine base	
B051095	Cocaine	Cocaine HCl	
B051114	Cocaine	Cocaine base + Phenacetin	
B051116	Cocaine	Cocaine HCl + Inositol	
B051118	Cocaine	Cocaine HCl	
B051119	Cocaine	Cocaine HCl	
B051120	Cocaine	Cocaine base	
B051124	Cocaine	Cocaine HCl	
B051129	Cocaine	Cocaine HCl	
B051130	Cocaine	Cocaine HCl	
B051134	Cocaine	Cocaine HCl	
B051159	Cocaine	Cocaine HCl + Inositol + Levamisole HCl	
B051165	Cocaine	Cocaine HCl + Inositol	
B051211	Cocaine	Cocaine HCl + Inositol	
B051213	Cocaine	Cocaine HCl	
B051214	Cocaine	Cocaine HCl	
B051215	Cocaine	Cocaine HCl	
B051216	Cocaine	Cocaine Base	
B051221	Cocaine	Cocaine HCl + Phenacetin	
B051223	Cocaine	Cocaine base + Phenacetin	
B051224	Cocaine	Cocaine Base	
B051226	Cocaine	Cocaine Base	
B051227	Cocaine	Cocaine HCl	
B051228	Cocaine	Cocaine HCl	
B051231	Cocaine	Cocaine Base	
B051232	Cocaine	Cocaine HCl	
B051233	Cocaine	Cocaine HCl	
B051235	Cocaine	Cocaine HCl	
B051239	Cocaine	Cocaine HCl	
B051240	Cocaine	Cocaine HCl	
B051254	Cocaine	Cocaine HCl	
B051255	Cocaine	Cocaine HCl	
B051256	Cocaine	Cocaine HCl	
B051258	Cocaine	Cocaine HCl	
B051264	Cocaine	Cocaine HCl	
B051265	Cocaine	Cocaine HCl	
B051266	Cocaine	Cocaine HCl	

**Table S1. (part 5 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B051279	Cocaine	Cocaine HCl	
B051284	Cocaine	Cocaine Base	
B051285	Cocaine	Cocaine Base	
B051293	Cocaine	Cocaine HCl	
B051294	Cocaine	Cocaine HCl	
B051295	Cocaine	Cocaine HCl	
B051297	Cocaine	Cocaine Base	
B051298	Cocaine	Cocaine HCl	
B051299	Cocaine	Cocaine HCl	
B051300	Cocaine	Cocaine HCl	
B051307	Cocaine	Cocaine HCl + Inositol	
B051313	Cocaine	Cocaine HCl + Levamisole HCl	
B051325	Cocaine	Cocaine HCl + Mannitol	
B051326	Cocaine	Cocaine HCl	
B051350	Cocaine	Cocaine Base	
B051355	Cocaine	Cocaine HCl	
B051357	Cocaine	Cocaine HCl + Inositol	
B051405	Cocaine	Cocaine HCl	
B051406	Cocaine	Cocaine HCl	
B051407	Cocaine	Cocaine HCl + Inositol	
B051411	Cocaine	Cocaine HCl	
B051496	Cocaine	Cocaine HCl + Inositol	
B051500	Cocaine	Cocaine base + Phenacetin	
B051501	Cocaine	Cocaine base + Phenacetin + Paracetamol	
B051504	Cocaine	Cocaine HCl	
B051506	Cocaine	Cocaine HCl + Lidocaine HCl	
B051517	Cocaine	Cocaine HCl	
B051523	Cocaine	Cocaine HCl + Inositol	
B051524	Cocaine	Cocaine HCl	
B051525	Cocaine	Cocaine HCl	
B051527	Cocaine	Cocaine HCl	
B051537	Cocaine	Cocaine HCl	
B051540	Cocaine	Cocaine HCl + Inositol	
B051541	Cocaine	Cocaine HCl	
B051542	Cocaine	Cocaine HCl	
B051543	Cocaine	Cocaine HCl + Inositol	
B051544	Cocaine	Cocaine Base	
B051549	Cocaine	Cocaine HCl	
B051551	Cocaine	Cocaine HCl	
B051553	Cocaine	Cocaine HCl	
B051565	Cocaine	Cocaine HCl + Phenacetin	
B051588	Cocaine	Cocaine Base	
B050732	Heroin	Heroin base	brown powder
B050800	Heroin	Inconclusive	brown powder
B050801	Heroin	Inconclusive	brown powder
B050836	Heroin	Caffeine + Paracetamol + Heroin base	brown powder
B050856	Heroin	Herione base	brown powder
B051069	Heroin	Heroin base	brown powder
B051283	Heroin	Paracetamol + Heroin Base	brown powder
B051497	Heroin	Paracetamol + Heroin Base	brown powder
B051499	Heroin	Paracetamol + Heroin Base	brown powder
B051545	Heroin	Paracetamol	brown powder
B050161	Ketamine	Ketamine	
B050255	Ketamine	Ketamine	
B050256	Ketamine	Ketamine	
B050315	Ketamine	Ketamine	
B050431	Ketamine	Ketamine	
B050470	Ketamine	Ketamine	
B050535	Ketamine	Ketamine	

**Table S1. (part 6 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050541	Ketamine	Ketamine	
B050546	Ketamine	Ketamine	
B050576	Ketamine	Ketamine	
B050691	Ketamine	Ketamine	
B050692	Ketamine	Ketamine	
B050693	Ketamine	Ketamine	
B050696	Ketamine	Ketamine	
B050702	Ketamine	Ketamine	
B050703	Ketamine	Ketamine	
B050704	Ketamine	Ketamine	
B050705	Ketamine	Ketamine	
B050707	Ketamine	Ketamine	
B050708	Ketamine	Ketamine	
B050709	Ketamine	Ketamine	
B050710	Ketamine	Ketamine	
B050712	Ketamine	Ketamine	
B050717	Ketamine	Ketamine	
B050719	Ketamine	Ketamine	
B050763	Ketamine	Ketamine	
B050775	Ketamine	Ketamine	
B050787	Ketamine	Ketamine	
B050863	Ketamine	Ketamine	
B050898	ketamine	Ketamine	
B051109	Ketamine	Ketamine	
B051117	Ketamine	Ketamine	
B051160	Ketamine	Ketamine	
B051238	Ketamine	Ketamine	
B051241	Ketamine	Ketamine	
B051260	Ketamine	Ketamine	
B051393	Ketamine	Ketamine	
B051394	Ketamine	Ketamine	
B051408	Ketamine	Ketamine	
B051412	Ketamine	Ketamine	
B051510	Ketamine	Ketamine	
B051518	Ketamine	Ketamine	
B051573	ketamine	ketamine	
B051586	Ketamine	ketamine	
B050531	MDMA	MDMA HCl	
B050533	MDMA	MDMA HCl	
B050575	MDMA	MDMA HCl	
B050689	MDMA	MDMA HCl	
B050694	MDMA	Cellulose + MDMA HCl	
B050700	MDMA	MDMA HCl	
B050701	MDMA	Cellulose + MDMA HCl	grey powder
B050714	MDMA	Cellulose + MDMA HCl	
B050715	MDMA	MDMA HCl	
B050716	MDMA	Cellulose + MDMA HCl	
B050727	MDMA	MDMA HCl	
B050728	MDMA	MDMA HCl	grey powder
B050764	MDMA	MDMA HCl	
B050770	MDMA	Inconclusive	grey powder
B050780	MDMA	MDMA HCl	
B050783	MDMA	Cellulose + MDMA HCl	orange powder
B050795	MDMA	MDMA HCl	pink powder
B050797	MDMA	MDMA HCl	pink powder
B050798	MDMA	Cellulose + MDMA HCl	orange/pink powder
B050799	MDMA	MDMA HCl	pink powder
B050838	MDMA	Cellulose + MDMA HCl	dark rood powder
B050839	MDMA	Inconclusive	dark green powder



**Table S1. (part 7 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050840	MDMA	Cellulose + MDMA HCl	green powder
B050841	MDMA	MDMA HCl	
B050842	MDMA	Cellulose + MDMA HCl	orange powder
B050847	MDMA	Cellulose + MDMA HCl	orange powder
B050855	MDMA	Inconclusive	blue-pink powder
B050867	MDMA	Cellulose + MDMA HCl	grey powder
B050879	MDMA	MDMA HCl	
B050882	MDMA	Cellulose + MDMA HCl	orange powder
B050893	MDMA	MDMA HCl	
B051113	MDMA	Cellulose + MDMA HCl	pink powder
B051128	MDMA	Cellulose + MDMA HCl	pink powder
B051131	MDMA	Cellulose + MDMA HCl	brown powder
B051133	MDMA	Cellulose + MDMA HCl	pink/purple powder
B051135	MDMA	Cellulose + MDMA HCl	light blue powder
B051145	MDMA	MDMA HCl	
B051168	MDMA	MDMA HCl	
B051170	MDMA	MDMA HCl + Cellulose	grey powder
B051171	MDMA	MDMA HCl	grey powder
B051212	MDMA	MDMA HCl	green powder
B051236	MDMA	MDMA HCl	beige powder
B051237	MDMA	MDMA HCl	
B051242	MDMA	Inconclusive	grey powder
B051249	MDMA	MDMA HCl	
B051250	MDMA	MDMA HCl	
B051253	MDMA	MDMA HCl	
B051259	MDMA	Cellulose + MDMA HCl	blue powder
B051262	MDMA	MDMA HCl	
B051263	MDMA	Cellulose + MDMA HCl	blue powder
B051271	MDMA	Cellulose + MDMA HCl	blue powder
B051276	MDMA	MDMA HCl	
B051311	MDMA	MDMA HCl	grey powder
B051346	MDMA	Inconclusive	mustard yellow
B051347	MDMA	MDMA HCl	
B051390	MDMA	Cellulose + MDMA HCl	pink powder
B051396	MDMA	MDMA HCl	
B051409	MDMA	MDMA HCl	
B051410	MDMA	MDMA HCl	purple powder
B051417	MDMA	Inconclusive	pink powder
B051505	MDMA	MDMA HCl	
B051507	MDMA	Cellulose + MDMA HCl	beige powder
B051509	MDMA	MDMA HCl	orange powder
B051530	MDMA	MDMA HCl	grey powder
B051531	MDMA	MDMA HCl	
B051533	MDMA	Cellulose + MDMA HCl	green powder
B051546	MDMA	Cellulose + MDMA HCl	green powder
B051547	MDMA	Inconclusive	black-brown powder
B051548	MDMA	MDMA HCl	
B051552	MDMA	MDMA HCl + Cellulose	brown powder
B051555	MDMA	MDMA HCl	
B051556	MDMA	Cellulose + MDMA HCl	brown powder
B051566	MDMA	Cellulose + MDMA HCl	yellow powder
B051567	MDMA	Cellulose + MDMA HCl	purple powder
B051572	MDMA	Cellulose + MDMA HCl	pink powder
B051577	MDMA	MDMA HCl	grey powder
B051580	MDMA	MDMA HCl	
B051585	MDMA	MDMA HCl	
B051267	MDMA + Ketamine	Ketamine	pink powder
B050781	MDMA + Ketamine	Ketamine + Methamphetamine	pink powder
B051132	MDMA + Ketamine	Inconclusive	salmon powder

**Table S1. (part 8 of 9) Comparison of GC-MS and NIR results for 516 casework samples**

code	result GC-MS	result NIR	remarks
B050782	MDMA + Ketamine	Ketamine + Methamphetamine	pink powder
B051419	Ketamine + MDMA + 2C-B	Inconclusive	pink powder
B051261	Ketamine	Ketamine + Methamphetamine	pink powder
B050322	Methadone	Inconclusive	
B050418	Methadone	Inconclusive	
B050419	Methadone	Inconclusive	
B050420	Methadone	Cellulose + Lactose	
B050421	Methadone	Cellulose + Lactose	
B050706	Methamphetamine	Methamphetamine	
B050711	Methamphetamine	Methamphetamine	
B050713	Methamphetamine	Methamphetamine	
B050784	Methamphetamine + Ketamine	Ketamine + Methamphetamine	
B050900	Methamphetamine	Methamphetamine	
B050901	Methamphetamine	Methamphetamine	
B051502	Methamphetamine	Methamphetamine	
B051511	Methamphetamine	Methamphetamine	
B051512	Methamphetamine	Methamphetamine	
B050511	N-ethyloripentedrone	Inconclusive	
B051413	N-ethyloripentedrone	Levamisole HCl	
B051415	N-ethyloripentedrone	3-MMC + 4-MEC + 2-FMA	
B050137	No drug detected	Inositol	
B050148	No drug detected	Inconclusive	
B050246	No drug detected	Cellulose	
B050417	No drug detected	Inconclusive	
B050574	No drug detected	Inconclusive	
B050729	No drug detected	Inconclusive	
B050731	No drug detected	Inconclusive	
B050751	No drug detected	Inconclusive	brown powder
B051048	No drug detected	Inconclusive	
B051049	No drug detected	Inconclusive	
B051050	No drug detected	Inconclusive	
B051122	No drug detected	Inconclusive	
B051125	No drug detected	Inconclusive	
B051140	No drug detected	Inconclusive	
B051148	No drug detected	Inconclusive	
B051155	No drug detected	Inconclusive	
B051157	No drug detected	Inconclusive	
B051161	No drug detected	Inconclusive	
B051163	No drug detected	Inconclusive	
B051217	No drug detected	Cellulose	blue powder
B051218	No drug detected	Cellulose	blue powder
B051229	No drug detected	Inconclusive	
B051230	No drug detected	Inconclusive	
B051534	No drug detected	Inconclusive	
B051535	No drug detected	Inconclusive	
B051563	No drug detected	Inconclusive	
B051398	Paracetamol	Paracetamol	
B051399	Paracetamol	Paracetamol	
B051234	Phenacetin	Phenacetin	
B050239	Lidocaine	Lidocaine base	
B050244	Lidocaine	Lidocaine base	
B051222	Lidocaine	Lidocaine base	
B051554	Lidocaine	Lidocaine HCl	

**Table S1. (part 9 of 9)** Comparison of GC-MS and NIR results for 516 casework samples

code	result GC-MS	result NIR	remarks
B050304	2-MMC	2-MMC + 3-MEC	
B050305	2-MMC	2-MMC + 3-MMC	
B050486	2-MMC	2-MMC	
B050487	2-MMC	2-MMC + 3-MMC	
B050496	2-MMC	2-MMC	
B050497	2-MMC	2-MMC	
B050590	2-MMC	2-MMC	
B051584	2-MMC	2-MMC + 3-MMC	
B051587	2-MMC	2-MMC + 4-MEC	
B050765	2C-B	Cellulose	yellow powder
B050786	2C-B	Cellulose + Mg stearaat	pink powder
B050865	2C-B	2C-B + Cellulose	pink powder
B050895	2C-B	Cellulose	pink powder
B051126	2C-B	Inconclusive	pink powder
B051275	2C-B	Cellulose + Mg stearaat	pink powder
B051328	2C-B	Cellulose + Mg stearaat	yellow powder
B051388	2C-B	Cellulose	yellow powder
B051404	2C-B	Cellulose	pink powder
B051529	2C-B	Cellulose	pink powder
B051569	2C-B	Cellulose	purple powder
B051570	2C-B	Cellulose	green powder
B051578	2C-B	Cellulose + Mg stearaat	yellow powder
B050312	3-MMC	3-MMC + 4-FMA	
B050313	3-MMC	3-MMC + 4-FMA	
B050316	3-MMC	3-MMC	
B050317	3-MMC	3-MMC	
B050407	3-MMC	3-MMC + 4-FMA	
B050408	3-MMC	3-MMC	
B050570	3-MMC	3-MMC	
B050695	3-MMC	3-MMC	
B050697	3-MMC	3-MMC	
B050698	3-MMC	3-MMC	
B050699	3-MMC	3-MMC	
B050776	3-MMC	3-MMC	
B050777	3-MMC	3-MMC	
B050788	3-MMC	3-MMC	
B051138	3-MMC	3-MMC + 2-MMC	
B051166	3-MMC	3-MMC + 4-MEC + 4-FMA	
B051167	3-MMC	3-MMC	
B051397	3-MMC	3-MMC + 4-MEC	
B051401	3-MMC	3-MMC	
B051402	3-MMC	3-MMC	
B051508	3-MMC	3-MMC	
B051575	3-MMC	3-MMC	
B051576	3-MMC	3-MMC + 4-FMA	
B051581	3-MMC	3-MMC + 4-MEC + 4-FMA	
B051582	3-MMC	3-MMC	
B050610	3-MMC + MDMA	3-MMC	
B050612	3-MMC + MDMA	3-MMC	minor peak MDMA
B050613	3-MMC + MDMA	3-MMC	minor peak MDMA
B050474	4-MMC	Inconclusive	NIR peak at 2000 nm (possible hydrate)
B050476	4-MMC	Inconclusive	NIR peak at 2000 nm (possible hydrate)

legend:

	correct result (true positive or true negative)
	false negative
	substance not in NIR library
	incorrect (not all drugs correct, wrong drug detected)