

Supplemental Information

for

Portable Near Infrared Spectroscopy for the Isomeric Differentiation of New Psychoactive Substances

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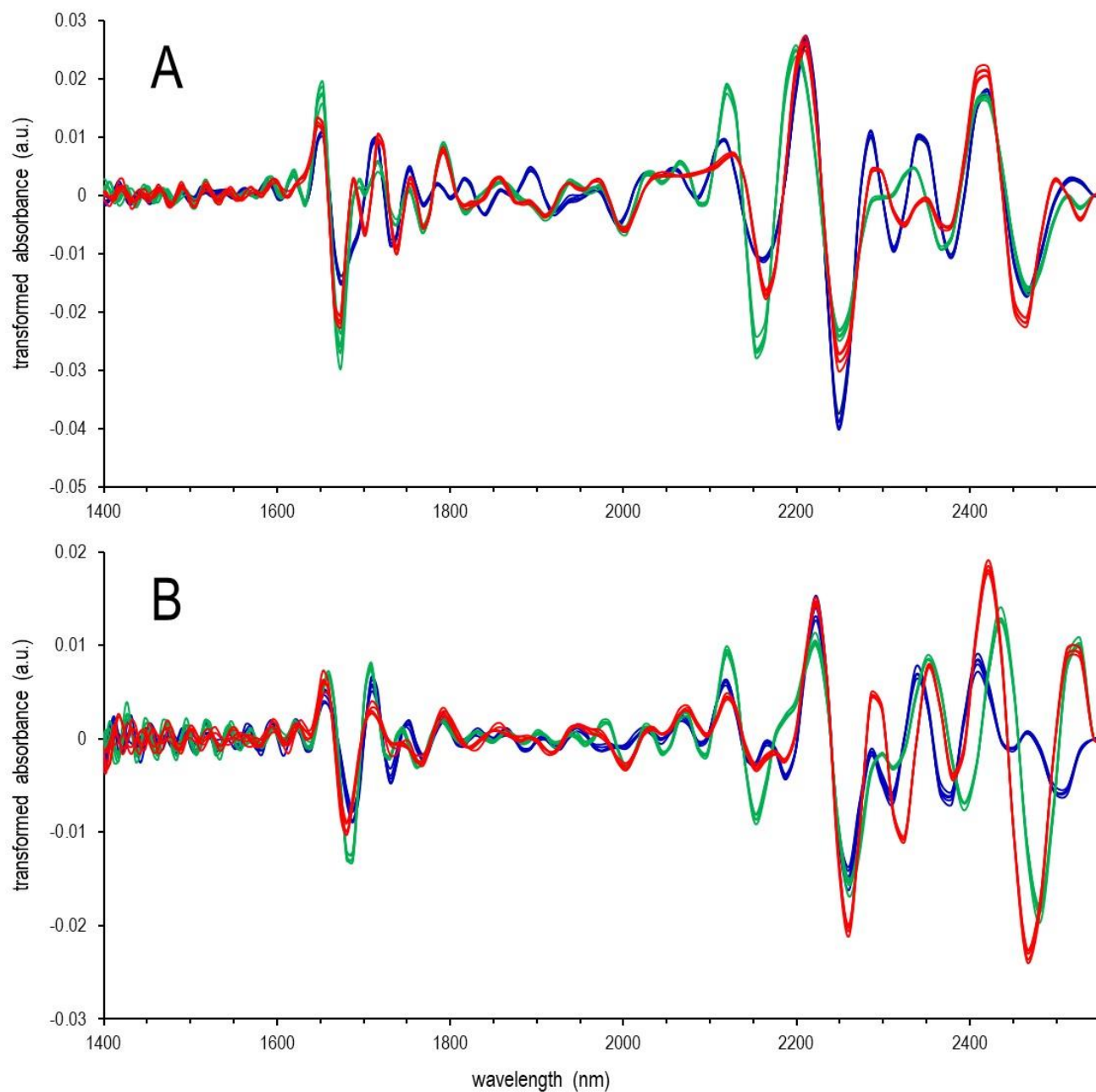


Figure S1. Second derivative NIR spectra of the cathinone isomeric sets shown in Figure 1; overlay of 5 replicate scans. Panel A: 2-MMC (blue), 3-MMC (green), 4-MMC (red); panel B: 2-MEC (blue), 3-MEC (green), and 4-MEC (red).

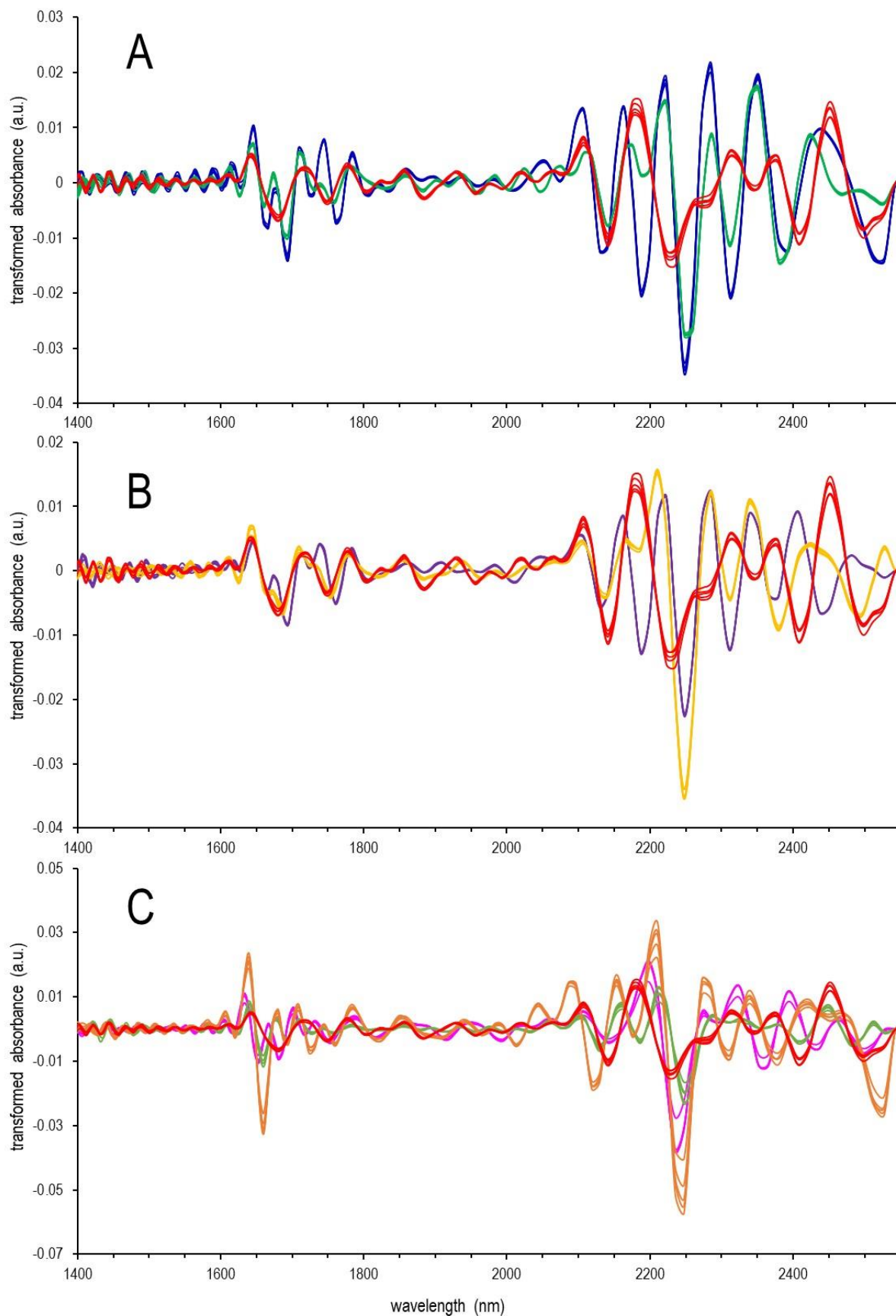


Figure S2. Second derivative NIR spectra of MDMA analogues shown in Figure 2; overlay of 5 replicate scans. 3,4-MDMA HCl (anhydrous) in red in all panels. Panel A: 3,4-MDA (blue), 3,4-MDEA (green); panel B: 2,3-MDA (purple), 2,3-MDMA (yellow); panel C: 2,3-methylone (pink), 3,4-methylone (orange), and 3,4-ethylone (dark green).

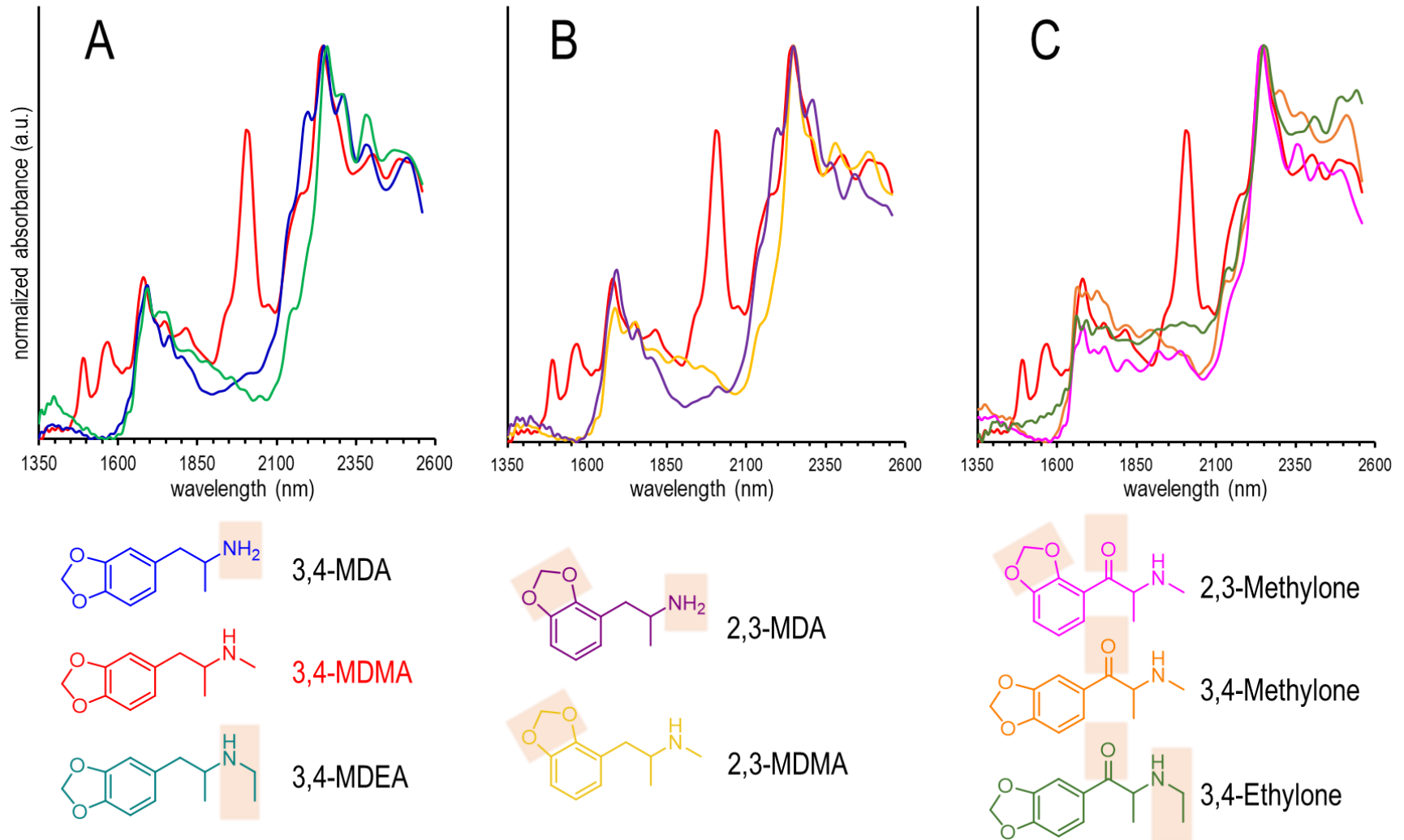


Figure S3. Normalized NIR spectra of MDMA analogues in overlay with 3,4-MDMA HCl (hydrated) in red in all panels. Panel A: 3,4-MDA (blue), 3,4-MDEA (green); panel B: 2,3-MDA (purple), 2,3-MDMA (yellow); panel C: 2,3-methylone (pink), 3,4-methylone (orange), and 3,4-ethylone (dark green). The orange shade in the molecular structures emphasizes the difference with MDMA.

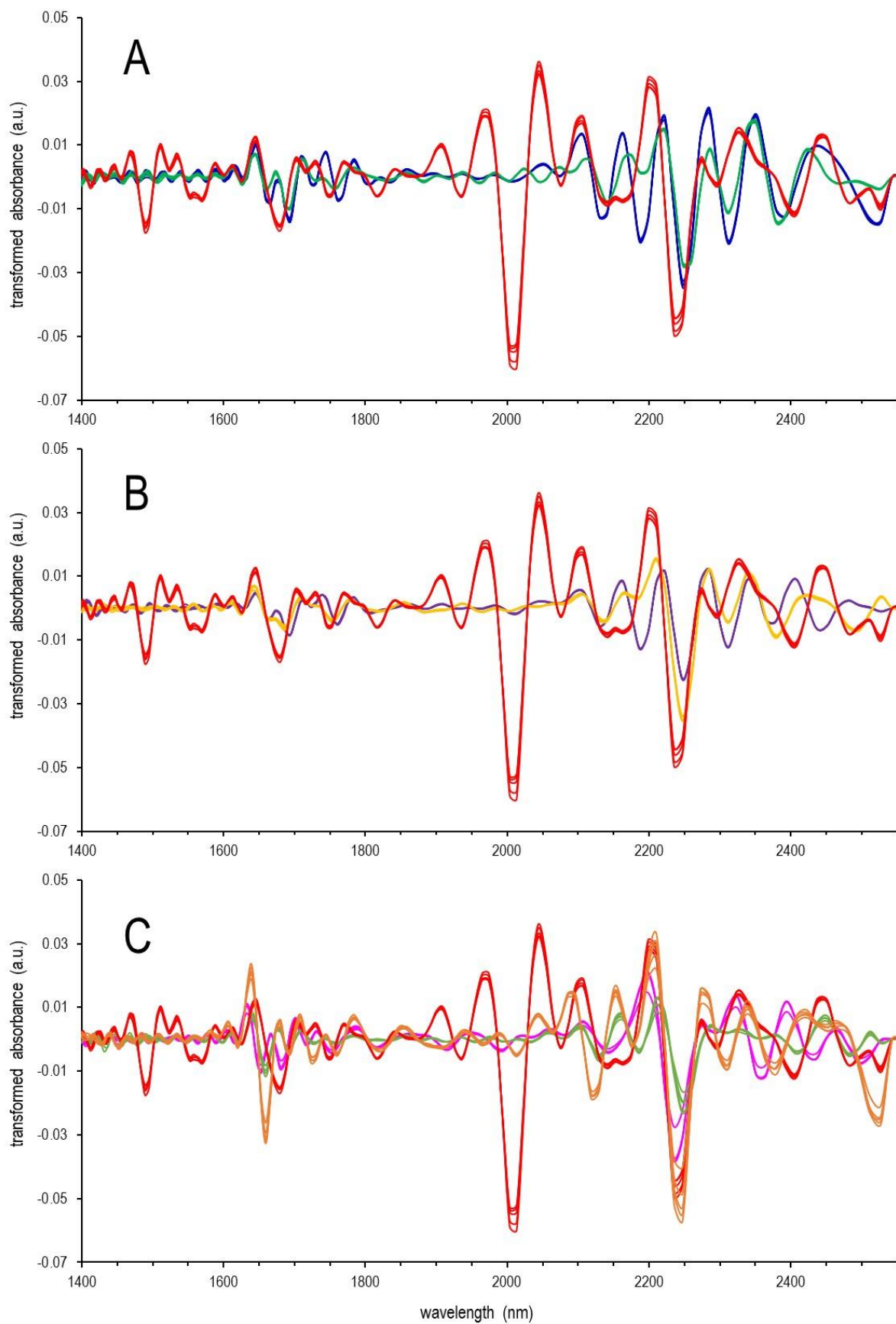


Figure S4. Second derivative NIR spectra of MDMA analogues shown in Figure S3; overlay of 5 replicate scans. 3,4-MDMA HCl (hydrated) in red in all panels. Panel A: 3,4-MDA (blue), 3,4-MDEA (green); panel B: 2,3-MDA (purple), 2,3-MDMA (yellow); panel C: 2,3-methylone (pink), 3,4-methylone (orange), and 3,4-ethylone (dark green).

Table S1. (part 1 of 4) Identification results of the 0 wt% - 100 wt% diluted cathinone mixtures.

Sample	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
microcrystalline cellulose 100%_1	Cellulose (98%)	0.98	Cellulose (98%)	0.98	Cellulose (98%)	0.98
microcrystalline cellulose 100%_2	Cellulose (98%)	0.98	Cellulose (98%)	0.98	Cellulose (98%)	0.98
microcrystalline cellulose 100%_3	Cellulose (99%)	0.99	Cellulose (99%)	0.99	Cellulose (99%)	0.99
microcrystalline cellulose 100%_4	Cellulose (97%)	0.97	Cellulose (97%)	0.97	Cellulose (97%)	0.97
microcrystalline cellulose 100%_5	Cellulose (98%)	0.98	Cellulose (98%)	0.98	Cellulose (98%)	0.98
microcrystalline cellulose 100%_6	Cellulose (98%)	0.98	Cellulose (98%)	0.98	Cellulose (98%)	0.98
2-MMC 10% in microcrystalline cellulose_1	2-MMC (21%) + Cellulose (76%)	0.97	2-MMC (21%) + Cellulose (76%)	0.97	2-MMC (21%) + Cellulose (76%)	0.97
2-MMC 10% in microcrystalline cellulose_2	2-MMC (21%) + Cellulose (76%)	0.96	2-MMC (21%) + Cellulose (76%)	0.96	2-MMC (21%) + Cellulose (76%)	0.96
2-MMC 10% in microcrystalline cellulose_3	2-MMC (22%) + Cellulose (73%)	0.95	2-MMC (22%) + Cellulose (73%)	0.95	2-MMC (22%) + Cellulose (73%)	0.95
2-MMC 20% in microcrystalline cellulose_1	2-MMC (30%) + Cellulose (66%)	0.96	2-MMC (31%) + Cellulose (64%)	0.96	2-MMC (30%) + Cellulose (66%)	0.96
2-MMC 20% in microcrystalline cellulose_2	2-MMC (30%) + Cellulose (66%)	0.96	2-MMC (30%) + Cellulose (66%)	0.96	2-MMC (30%) + Cellulose (66%)	0.96
2-MMC 20% in microcrystalline cellulose_3	2-MMC (28%) + Cellulose (67%)	0.95	2-MMC (28%) + Cellulose (67%)	0.95	2-MMC (28%) + Cellulose (67%)	0.95
2-MMC 30% in microcrystalline cellulose_1	2-MMC (41%) + Cellulose (54%)	0.95	2-MMC (41%) + Cellulose (54%)	0.95	2-MMC (41%) + Cellulose (55%)	0.95
2-MMC 30% in microcrystalline cellulose_2	2-MMC (40%) + Cellulose (57%)	0.96	2-MMC (39%) + Cellulose (57%)	0.96	2-MMC (39%) + Cellulose (57%)	0.96
2-MMC 30% in microcrystalline cellulose_3	2-MMC (40%) + Cellulose (55%)	0.95	2-MMC (40%) + Cellulose (55%)	0.95	2-MMC (40%) + Cellulose (55%)	0.95
2-MMC 40% in microcrystalline cellulose_1	2-MMC (50%) + Cellulose (44%)	0.94	2-MMC (50%) + Cellulose (44%)	0.94	2-MMC (50%) + Cellulose (44%)	0.94
2-MMC 40% in microcrystalline cellulose_2	2-MMC (47%) + Cellulose (46%)	0.93	2-MMC (47%) + Cellulose (46%)	0.93	2-MMC (47%) + Cellulose (46%)	0.93
2-MMC 40% in microcrystalline cellulose_3	2-MMC (48%) + Cellulose (48%)	0.95	2-MMC (48%) + Cellulose (48%)	0.95	2-MMC (48%) + Cellulose (48%)	0.95
2-MMC 50% in microcrystalline cellulose_1	2-MMC (54%) + Cellulose (42%)	0.96	2-MMC (54%) + Cellulose (42%)	0.96	2-MMC (54%) + Cellulose (42%)	0.96
2-MMC 50% in microcrystalline cellulose_2	2-MMC (56%) + Cellulose (39%)	0.95	2-MMC (51%) + Cellulose (32%)	0.95	2-MMC (49%) + Cellulose (35%)	0.95
2-MMC 50% in microcrystalline cellulose_3	2-MMC (54%) + Cellulose (42%)	0.96	2-MMC (48%) + Cellulose (37%)	0.96	2-MMC (54%) + Cellulose (42%)	0.96
2-MMC 60% in microcrystalline cellulose_1	2-MMC (55%) + Cellulose (29%)	0.95	2-MMC (57%) + Cellulose (27%)	0.95	2-MMC (55%) + Cellulose (29%)	0.95
2-MMC 60% in microcrystalline cellulose_2	2-MMC (58%) + Cellulose (29%)	0.97	2-MMC (57%) + Cellulose (29%)	0.96	2-MMC (58%) + Cellulose (28%)	0.96
2-MMC 60% in microcrystalline cellulose_3	2-MMC (57%) + Cellulose (28%)	0.95	2-MMC (58%) + Cellulose (25%)	0.95	2-MMC (57%) + Cellulose (28%)	0.95
2-MMC 70% in microcrystalline cellulose_1	2-MMC (63%) + Cellulose (22%)	0.96	2-MMC (73%) + Cellulose (23%)	0.96	2-MMC (62%) + Cellulose (23%)	0.96
2-MMC 70% in microcrystalline cellulose_2	2-MMC (63%) + Cellulose (23%)	0.96	2-MMC (63%) + Cellulose (23%)	0.96	2-MMC (64%) + Cellulose (22%)	0.96
2-MMC 70% in microcrystalline cellulose_3	2-MMC (65%) + Cellulose (22%)	0.97	2-MMC (64%) + Cellulose (23%)	0.97	2-MMC (65%) + Cellulose (22%)	0.97
2-MMC 80% in microcrystalline cellulose_1	2-MMC (71%) + Cellulose (17%)	0.97	2-MMC (69%) + Cellulose (19%)	0.97	2-MMC (69%) + Cellulose (18%)	0.97
2-MMC 80% in microcrystalline cellulose_2	2-MMC (65%) + Cellulose (18%)	0.95	2-MMC (66%) + Cellulose (17%)	0.95	2-MMC (65%) + Cellulose (18%)	0.95
2-MMC 80% in microcrystalline cellulose_3	2-MMC (68%) + Cellulose (17%)	0.95	2-MMC (69%) + Cellulose (17%)	0.95	2-MMC (68%) + Cellulose (17%)	0.95
2-MMC 90% in microcrystalline cellulose_1	2-MMC (79%) + Cellulose (10%)	0.97	2-MMC (79%) + Cellulose (10%)	0.97	2-MMC (78%) + Cellulose (10%)	0.97
2-MMC 90% in microcrystalline cellulose_2	2-MMC (80%) + Cellulose (11%)	0.98	2-MMC (81%) + Cellulose (10%)	0.98	2-MMC (80%) + Cellulose (11%)	0.98
2-MMC 90% in microcrystalline cellulose_3	2-MMC (78%) + Cellulose (11%)	0.97	2-MMC (78%) + Cellulose (11%)	0.97	2-MMC (78%) + Cellulose (11%)	0.97
2-MMC 100%_1	2-MMC (82%)	0.97	2-MMC (97%)	0.97	2-MMC (97%)	0.97
2-MMC 100%_2	2-MMC (81%)	0.96	2-MMC (95%)	0.95	2-MMC (96%)	0.96
2-MMC 100%_3	2-MMC (81%)	0.96	2-MMC (81%)	0.96	2-MMC (80%)	0.96

Note. Results in **red** indicate erroneous identifications, results in **gray** on library options 2 (multiple drug allowed) and 3 (including both hydrated and anhydrous 4-MMC) are presented for information only.

Table S1. (part 2 of 4) Identification results of the 0 wt% - 100 wt% diluted cathinone mixtures.

Sample	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
3-MMC 10% in microcrystalline cellulose_1	3-MMC (14%) + Cellulose (82%)	0.96	3-MMC (14%) + Cellulose (82%)	0.96	3-MMC (14%) + Cellulose (83%)	0.96
3-MMC 10% in microcrystalline cellulose_2	3-MMC (13%) + Cellulose (85%)	0.98	3-MMC (13%) + Cellulose (84%)	0.98	3-MMC (13%) + Cellulose (84%)	0.98
3-MMC 10% in microcrystalline cellulose_3	3-MMC (14%) + Cellulose (84%)	0.98	3-MMC (14%) + Cellulose (84%)	0.98	3-MMC (14%) + Cellulose (84%)	0.98
3-MMC 20% in microcrystalline cellulose_1	3-MMC (23%) + Cellulose (73%)	0.97	3-MMC (23%) + Cellulose (73%)	0.97	3-MMC (24%) + Cellulose (73%)	0.97
3-MMC 20% in microcrystalline cellulose_2	3-MMC (23%) + Cellulose (73%)	0.96	3-MMC (23%) + Cellulose (73%)	0.96	3-MMC (23%) + Cellulose (73%)	0.96
3-MMC 20% in microcrystalline cellulose_3	3-MMC (25%) + Cellulose (72%)	0.96	3-MMC (25%) + Cellulose (72%)	0.96	3-MMC (25%) + Cellulose (72%)	0.97
3-MMC 30% in microcrystalline cellulose_1	3-MMC (45%) + Cellulose (39%)	0.95	3-MMC (45%) + Cellulose (39%)	0.95	3-MMC (45%) + Cellulose (39%)	0.95
3-MMC 30% in microcrystalline cellulose_2	3-MMC (34%) + Cellulose (63%)	0.96	3-MMC (34%) + Cellulose (63%)	0.96	3-MMC (34%) + Cellulose (63%)	0.97
3-MMC 30% in microcrystalline cellulose_3	3-MMC (34%) + Cellulose (62%)	0.96	3-MMC (34%) + Cellulose (63%)	0.96	3-MMC (34%) + Cellulose (62%)	0.96
3-MMC 40% in microcrystalline cellulose_1	3-MMC (38%) + Cellulose (57%)	0.95	3-MMC (38%) + Cellulose (57%)	0.95	3-MMC (38%) + Cellulose (57%)	0.95
3-MMC 40% in microcrystalline cellulose_2	3-MMC (40%) + Cellulose (55%)	0.95	3-MMC (40%) + Cellulose (55%)	0.95	3-MMC (40%) + Cellulose (55%)	0.95
3-MMC 40% in microcrystalline cellulose_3	3-MMC (35%) + Cellulose (51%)	0.96	3-MMC (35%) + Cellulose (51%)	0.96	3-MMC (39%) + Cellulose (57%)	0.96
3-MMC 50% in microcrystalline cellulose_1	3-MMC (46%) + Cellulose (36%)	0.94	3-MMC (46%) + Cellulose (36%)	0.94	3-MMC (46%) + Cellulose (36%)	0.94
3-MMC 50% in microcrystalline cellulose_2	3-MMC (49%) + Cellulose (47%)	0.95	3-MMC (44%) + Cellulose (42%)	0.95	3-MMC (49%) + Cellulose (47%)	0.95
3-MMC 50% in microcrystalline cellulose_3	3-MMC (44%) + Cellulose (42%)	0.96	3-MMC (44%) + Cellulose (42%)	0.96	3-MMC (44%) + Cellulose (42%)	0.96
3-MMC 60% in microcrystalline cellulose_1	3-MMC (50%) + Cellulose (34%)	0.95	3-MMC (50%) + Cellulose (34%)	0.95	3-MMC (50%) + Cellulose (34%)	0.95
3-MMC 60% in microcrystalline cellulose_2	3-MMC (52%) + Cellulose (34%)	0.95	3-MMC (50%) + Cellulose (35%)	0.95	3-MMC (50%) + Cellulose (35%)	0.95
3-MMC 60% in microcrystalline cellulose_3	3-MMC (49%) + Cellulose (35%)	0.94	3-MMC (49%) + Cellulose (35%)	0.95	3-MMC (48%) + Cellulose (36%)	0.94
3-MMC 70% in microcrystalline cellulose_1	3-MMC (57%) + Cellulose (26%)	0.94	3-MMC (57%) + Cellulose (26%)	0.94	3-MMC (57%) + Cellulose (26%)	0.94
3-MMC 70% in microcrystalline cellulose_2	3-MMC (60%) + Cellulose (24%)	0.95	3-MMC (60%) + Cellulose (24%)	0.95	3-MMC (61%) + Cellulose (24%)	0.95
3-MMC 70% in microcrystalline cellulose_3	3-MMC (54%) + Cellulose (29%)	0.94	3-MMC (54%) + Cellulose (29%)	0.94	3-MMC (55%) + Cellulose (29%)	0.94
3-MMC 80% in microcrystalline cellulose_1	3-MMC (72%) + Cellulose (15%)	0.97	3-MMC (72%) + Cellulose (15%)	0.96	3-MMC (72%) + Cellulose (15%)	0.97
3-MMC 80% in microcrystalline cellulose_2	3-MMC (66%) + Cellulose (19%)	0.95	3-MMC (66%) + Cellulose (19%)	0.95	3-MMC (66%) + Cellulose (19%)	0.95
3-MMC 80% in microcrystalline cellulose_3	3-MMC (65%) + Cellulose (19%)	0.96	3-MMC (65%) + Cellulose (20%)	0.96	3-MMC (66%) + Cellulose (20%)	0.96
3-MMC 90% in microcrystalline cellulose_1	3-MMC (78%) + Cellulose (10%)	0.97	3-MMC (73%)	0.95	3-MMC (77%) + Cellulose (10%)	0.97
3-MMC 90% in microcrystalline cellulose_2	3-MMC (80%) + Cellulose (10%)	0.98	3-MMC (76%)	0.97	3-MMC (80%) + Cellulose (10%)	0.98
3-MMC 90% in microcrystalline cellulose_3	3-MMC (76%) + Cellulose (11%)	0.96	3-MMC (71%)	0.95	3-MMC (76%) + Cellulose (10%)	0.96
3-MMC 100%_1	3-MMC (97%)	0.97	3-MMC (81%)	0.97	3-MMC (81%)	0.97
3-MMC 100%_2	3-MMC (98%)	0.98	3-MMC (84%)	0.98	3-MMC (98%)	0.98
3-MMC 100%_3	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98

Note. Results in **red** indicate erroneous identifications, results in **gray** on library options 2 (multiple drug allowed) and 3 (including both hydrated and anhydrous 4-MMC) are presented for information only.

Table S1. (part 3 of 4) Identification results of the 0 wt% - 100 wt% diluted cathinone mixtures.

Sample	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
4-MMC 10% in microcrystalline cellulose_1	4-MMC anhydrate (12%) + Cellulose (84%)	0.97	4-MMC anhydrate (12%) + Cellulose (84%)	0.97	4-MMC anhydrate (12%) + Cellulose (84%)	0.97
4-MMC 10% in microcrystalline cellulose_2	4-MMC anhydrate (11%) + Cellulose (86%)	0.97	4-MMC anhydrate (11%) + Cellulose (86%)	0.97	4-MMC anhydrate (11%) + Cellulose (86%)	0.97
4-MMC 10% in microcrystalline cellulose_3	4-MMC anhydrate (11%) + Cellulose (86%)	0.97	4-MMC anhydrate (11%) + Cellulose (86%)	0.97	4-MMC anhydrate (11%) + Cellulose (86%)	0.97
4-MMC 20% in microcrystalline cellulose_1	4-MMC anhydrate (23%) + Cellulose (73%)	0.96	4-MMC anhydrate (23%) + Cellulose (73%)	0.96	4-MMC anhydrate (23%) + Cellulose (73%)	0.96
4-MMC 20% in microcrystalline cellulose_2	4-MMC anhydrate (23%) + Cellulose (74%)	0.97	4-MMC anhydrate (22%) + Cellulose (74%)	0.97	4-MMC anhydrate (22%) + Cellulose (74%)	0.97
4-MMC 20% in microcrystalline cellulose_3	4-MMC anhydrate (22%) + Cellulose (74%)	0.97	4-MMC anhydrate (22%) + Cellulose (74%)	0.97	4-MMC anhydrate (23%) + Cellulose (74%)	0.97
4-MMC 30% in microcrystalline cellulose_1	4-MMC anhydrate (34%) + Cellulose (62%)	0.97	4-MMC anhydrate (34%) + Cellulose (63%)	0.97	4-MMC anhydrate (34%) + Cellulose (62%)	0.97
4-MMC 30% in microcrystalline cellulose_2	4-MMC anhydrate (33%) + Cellulose (65%)	0.97	4-MMC anhydrate (23%) + 2-MMC (15%) + Cellulose (60%)	0.97	4-MMC anhydrate (33%) + Cellulose (65%)	0.97
4-MMC 30% in microcrystalline cellulose_3	4-MMC anhydrate (31%) + Cellulose (65%)	0.96	4-MMC anhydrate (31%) + Cellulose (65%)	0.96	4-MMC anhydrate (31%) + Cellulose (65%)	0.96
4-MMC 40% in microcrystalline cellulose_1	4-MMC anhydrate (36%) + Cellulose (61%)	0.97	4-MMC anhydrate (36%) + Cellulose (61%)	0.97	4-MMC anhydrate (36%) + Cellulose (61%)	0.97
4-MMC 40% in microcrystalline cellulose_2	4-MMC anhydrate (39%) + Cellulose (47%)	0.95	4-MMC anhydrate (30%) + 2-MMC (18%) + Cellulose (48%)	0.96	4-MMC anhydrate (39%) + Cellulose (47%)	0.95
4-MMC 40% in microcrystalline cellulose_3	4-MMC anhydrate (37%) + Cellulose (48%)	0.95	4-MMC anhydrate (37%) + Cellulose (48%)	0.95	4-MMC anhydrate (37%) + Cellulose (48%)	0.95
4-MMC 50% in microcrystalline cellulose_1	4-MMC anhydrate (40%) + Cellulose (56%)	0.96	4-MMC anhydrate (40%) + Cellulose (57%)	0.96	4-MMC anhydrate (40%) + Cellulose (57%)	0.96
4-MMC 50% in microcrystalline cellulose_2	4-MMC anhydrate (46%) + Cellulose (41%)	0.96	4-MMC anhydrate (41%) + Cellulose (44%)	0.96	4-MMC anhydrate (46%) + Cellulose (41%)	0.96
4-MMC 50% in microcrystalline cellulose_3	4-MMC anhydrate (43%) + Cellulose (41%)	0.95	4-MMC anhydrate (43%) + Cellulose (41%)	0.95	4-MMC anhydrate (43%) + Cellulose (41%)	0.94
4-MMC 60% in microcrystalline cellulose_1	4-MMC anhydrate (45%) + Cellulose (40%)	0.95	4-MMC anhydrate (45%) + Cellulose (40%)	0.95	4-MMC anhydrate (45%) + Cellulose (40%)	0.95
4-MMC 60% in microcrystalline cellulose_2	4-MMC anhydrate (51%) + Cellulose (34%)	0.95	4-MMC anhydrate (51%) + Cellulose (34%)	0.95	4-MMC anhydrate (51%) + Cellulose (33%)	0.95
4-MMC 60% in microcrystalline cellulose_3	4-MMC anhydrate (50%) + Cellulose (35%)	0.96	4-MMC anhydrate (50%) + Cellulose (35%)	0.96	4-MMC anhydrate (50%) + Cellulose (35%)	0.96
4-MMC 70% in microcrystalline cellulose_1	4-MMC anhydrate (53%) + Cellulose (28%)	0.93	4-MMC anhydrate (52%) + Cellulose (28%)	0.93	4-MMC anhydrate (53%) + Cellulose (28%)	0.93
4-MMC 70% in microcrystalline cellulose_2	4-MMC anhydrate (58%) + Cellulose (26%)	0.95	4-MMC anhydrate (58%) + Cellulose (26%)	0.95	4-MMC anhydrate (58%) + Cellulose (26%)	0.95
4-MMC 70% in microcrystalline cellulose_3	4-MMC anhydrate (55%) + Cellulose (28%)	0.94	4-MMC anhydrate (52%) + Cellulose (30%)	0.94	4-MMC anhydrate (55%) + Cellulose (28%)	0.94
4-MMC 80% in microcrystalline cellulose_1	4-MMC anhydrate (67%) + Cellulose (21%)	0.97	4-MMC anhydrate (68%) + Cellulose (20%)	0.97	4-MMC anhydrate (67%) + Cellulose (21%)	0.97
4-MMC 80% in microcrystalline cellulose_2	4-MMC anhydrate (64%) + Cellulose (20%)	0.95	4-MMC anhydrate (64%) + Cellulose (20%)	0.95	4-MMC anhydrate (64%) + Cellulose (20%)	0.95
4-MMC 80% in microcrystalline cellulose_3	4-MMC anhydrate (66%) + Cellulose (19%)	0.95	4-MMC anhydrate (65%) + Cellulose (19%)	0.95	4-MMC anhydrate (66%) + Cellulose (19%)	0.95
4-MMC 90% in microcrystalline cellulose_1	4-MMC anhydrate (77%) + Cellulose (10%)	0.96	4-MMC anhydrate (78%) + Cellulose (10%)	0.96	4-MMC anhydrate (77%) + Cellulose (10%)	0.96
4-MMC 90% in microcrystalline cellulose_2	4-MMC anhydrate (77%) + Cellulose (9%)	0.96	4-MMC anhydrate (76%) + Cellulose (10%)	0.95	4-MMC anhydrate (77%) + Cellulose (9%)	0.96
4-MMC 90% in microcrystalline cellulose_3	4-MMC anhydrate (77%) + Cellulose (9%)	0.96	4-MMC anhydrate (77%) + Cellulose (10%)	0.96	4-MMC anhydrate (77%) + Cellulose (9%)	0.96
4-MMC 100% _1	4-MMC anhydrate (78%)	0.96	4-MMC anhydrate (77%)	0.96	4-MMC anhydrate (78%)	0.96
4-MMC 100% _2	4-MMC anhydrate (77%)	0.96	4-MMC anhydrate (76%)	0.96	4-MMC anhydrate (76%)	0.96
4-MMC 100% _3	4-MMC anhydrate (76%)	0.96	4-MMC anhydrate (76%)	0.96	4-MMC anhydrate (76%)	0.96

Note. Results in **red** indicate erroneous identifications, results in **gray** on library options 2 (multiple drug allowed) and 3 (including both hydrated and anhydrous 4-MMC) are presented for information only.

Table S1. (part 4 of 4) Identification results of the 0 wt% - 100 wt% diluted cathinone mixtures.

Sample	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
4-MEC 10% in microcrystalline cellulose_1	2-MEC (11%) + Cellulose (86%)	0.98	2-MEC (11%) + Cellulose (87%)	0.98	4-MEC (12%) + Cellulose (86%)	0.98
4-MEC 10% in microcrystalline cellulose_2	4-MEC (12%) + Cellulose (84%)	0.96	2-MEC (10%) + Cellulose (79%)	0.97	2-MEC (11%) + Cellulose (86%)	0.97
4-MEC 10% in microcrystalline cellulose_3	4-MEC (13%) + Cellulose (85%)	0.98	4-MEC (13%) + Cellulose (85%)	0.98	4-MEC (13%) + Cellulose (85%)	0.98
4-MEC 20% in microcrystalline cellulose_1	4-MEC (22%) + Cellulose (73%)	0.95	4-MEC (22%) + Cellulose (73%)	0.95	4-MEC (22%) + Cellulose (73%)	0.95
4-MEC 20% in microcrystalline cellulose_2	4-MEC (24%) + Cellulose (72%)	0.96	4-MEC (24%) + Cellulose (72%)	0.96	4-MEC (24%) + Cellulose (72%)	0.96
4-MEC 20% in microcrystalline cellulose_3	4-MEC (21%) + Cellulose (73%)	0.94	4-MEC (21%) + Cellulose (73%)	0.94	4-MEC (21%) + Cellulose (73%)	0.95
4-MEC 30% in microcrystalline cellulose_1	4-MEC (31%) + Cellulose (64%)	0.95	4-MEC (28%) + Cellulose (58%)	0.95	4-MEC (28%) + Cellulose (58%)	0.95
4-MEC 30% in microcrystalline cellulose_2	4-MEC (30%) + Cellulose (67%)	0.97	4-MEC (30%) + Cellulose (67%)	0.97	4-MEC (30%) + Cellulose (67%)	0.97
4-MEC 30% in microcrystalline cellulose_3	4-MEC (28%) + Cellulose (58%)	0.96	4-MEC (28%) + Cellulose (58%)	0.95	4-MEC (28%) + Cellulose (58%)	0.95
4-MEC 40% in microcrystalline cellulose_1	4-MEC (35%) + Cellulose (48%)	0.94	4-MEC (39%) + Cellulose (54%)	0.94	4-MEC (35%) + Cellulose (48%)	0.93
4-MEC 40% in microcrystalline cellulose_2	4-MEC (42%) + Cellulose (51%)	0.93	4-MEC (37%) + Cellulose (45%)	0.93	4-MEC (37%) + Cellulose (45%)	0.93
4-MEC 40% in microcrystalline cellulose_3	4-MEC (39%) + Cellulose (47%)	0.96	4-MEC (39%) + Cellulose (47%)	0.96	4-MEC (39%) + Cellulose (47%)	0.96
4-MEC 50% in microcrystalline cellulose_1	4-MEC (44%) + Cellulose (41%)	0.96	4-MEC (44%) + Cellulose (41%)	0.96	4-MEC (44%) + Cellulose (41%)	0.96
4-MEC 50% in microcrystalline cellulose_2	4-MEC (45%) + Cellulose (48%)	0.93	4-MEC (45%) + Cellulose (48%)	0.93	4-MEC (45%) + Cellulose (48%)	0.93
4-MEC 50% in microcrystalline cellulose_3	4-MEC (43%) + Cellulose (40%)	0.94	4-MEC (43%) + Cellulose (40%)	0.94	4-MEC (43%) + Cellulose (40%)	0.94
4-MEC 60% in microcrystalline cellulose_1	4-MEC (53%) + Cellulose (42%)	0.95	4-MEC (55%) + Cellulose (40%)	0.95	4-MEC (53%) + Cellulose (42%)	0.95
4-MEC 60% in microcrystalline cellulose_2	4-MEC (55%) + Cellulose (42%)	0.97	4-MEC (49%) + Cellulose (38%)	0.97	4-MEC (55%) + Cellulose (42%)	0.97
4-MEC 60% in microcrystalline cellulose_3	4-MEC (52%) + Cellulose (36%)	0.97	4-MEC (51%) + Cellulose (37%)	0.97	4-MEC (52%) + Cellulose (36%)	0.97
4-MEC 70% in microcrystalline cellulose_1	4-MEC (67%) + Cellulose (29%)	0.96	4-MEC (60%) + Cellulose (26%)	0.96	4-MEC (67%) + Cellulose (29%)	0.96
4-MEC 70% in microcrystalline cellulose_2	4-MEC (64%) + Cellulose (33%)	0.97	4-MEC (58%) + Cellulose (30%)	0.97	4-MEC (64%) + Cellulose (33%)	0.97
4-MEC 70% in microcrystalline cellulose_3	4-MEC (64%) + Cellulose (32%)	0.96	4-MEC (58%) + Cellulose (28%)	0.96	4-MEC (64%) + Cellulose (32%)	0.96
4-MEC 80% in microcrystalline cellulose_1	4-MEC (76%) + Cellulose (23%)	0.99	4-MEC (71%) + Cellulose (21%)	0.99	4-MEC (76%) + Cellulose (23%)	0.99
4-MEC 80% in microcrystalline cellulose_2	4-MEC (75%) + Cellulose (22%)	0.98	4-MEC (77%) + Cellulose (21%)	0.98	4-MEC (75%) + Cellulose (22%)	0.98
4-MEC 80% in microcrystalline cellulose_3	4-MEC (76%) + Cellulose (21%)	0.97	4-MEC (71%) + Cellulose (18%)	0.97	4-MEC (76%) + Cellulose (21%)	0.97
4-MEC 90% in microcrystalline cellulose_1	4-MEC (87%) + Cellulose (11%)	0.97	4-MEC (87%) + Cellulose (10%)	0.97	4-MEC (87%) + Cellulose (11%)	0.97
4-MEC 90% in microcrystalline cellulose_2	4-MEC (88%) + Cellulose (11%)	0.98	4-MEC (88%) + Cellulose (11%)	0.98	4-MEC (87%) + Cellulose (11%)	0.98
4-MEC 90% in microcrystalline cellulose_3	4-MEC (85%) + Cellulose (13%)	0.98	4-MEC (86%) + Cellulose (12%)	0.98	4-MEC (85%) + Cellulose (13%)	0.98
4-MEC 100% _1	4-MEC (97%)	0.97	4-MEC (97%)	0.97	4-MEC (97%)	0.97
4-MEC 100% _2	4-MEC (98%)	0.98	4-MEC (98%)	0.98	4-MEC (98%)	0.98
4-MEC 100% _3	4-MEC (96%)	0.96	4-MEC (96%)	0.96	4-MEC (95%)	0.95

Note. Results in **red** indicate erroneous identifications, results in **gray** on library options 2 (multiple drug allowed) and 3 (including both hydrated and anhydrous 4-MMC) are presented for information only.

Table S2. Identification results of the cathinone drug-isomer mixtures.

Sample	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
2-MMC : 3-MMC, 50:50_1	2-MMC (61%)	0.91	2-MMC (55%) + 3-MMC (34%)	0.96	2-MMC (61%)	0.91
2-MMC : 3-MMC, 50:50_2	2-MMC (58%)	0.90	2-MMC (51%) + 3-MMC (36%)	0.95	2-MMC (58%)	0.90
2-MMC : 3-MMC, 50:50_3	2-MMC (61%)	0.92	2-MMC (52%) + 3-MMC (37%)	0.97	2-MMC (61%)	0.92
2-MMC : 3-MMC, 75:25_1	2-MMC (91%) + Cellulose (6%)	0.96	2-MMC (79%) + 3-MMC (13%) + Cellulose (5%)	0.97	2-MMC (91%) + Cellulose (6%)	0.96
2-MMC : 3-MMC, 75:25_2	2-MMC (91%) + Cellulose (6%)	0.96	2-MMC (80%) + 3-MMC (16%)	0.97	2-MMC (91%) + Cellulose (6%)	0.96
2-MMC : 3-MMC, 75:25_3	2-MMC (90%) + Cellulose (6%)	0.96	2-MMC (90%) + Cellulose (6%)	0.96	2-MMC (91%) + Cellulose (6%)	0.97
2-MMC : 4-MEC, 50:50_1	4-MEC (49%)	0.83	2-MMC (53%) + 4-MEC (40%)	0.93	4-MEC (51%)	0.83
2-MMC : 4-MEC, 50:50_2	4-MEC (53%)	0.86	2-MMC (54%) + 4-MEC (40%)	0.94	4-MEC (54%)	0.86
2-MMC : 4-MEC, 50:50_3	4-MEC (50%)	0.84	2-MMC (54%) + 4-MEC (38%)	0.92	4-MEC (50%)	0.84
2-MMC : 4-MEC, 75:25_1	2-MMC (61%)	0.90	2-MMC (69%) + 4-MEC (24%)	0.93	2-MMC (60%)	0.90
2-MMC : 4-MEC, 75:25_2	2-MMC (63%)	0.93	2-MMC (72%) + 4-MEC (22%)	0.94	2-MMC (64%)	0.93
2-MMC : 4-MEC, 75:25_3	2-MMC (63%)	0.92	2-MMC (73%) + 4-MEC (22%)	0.95	2-MMC (64%)	0.92
2-MMC : 4-MMC, 50:50_1	2-MMC (53%)	0.87	2-MMC (40%) + 4-MMC anhydrate (44%)	0.94	2-MMC (53%)	0.87
2-MMC : 4-MMC, 50:50_2	2-MMC (57%)	0.88	2-MMC (54%) + 4-MMC anhydrate (42%)	0.96	2-MMC (57%)	0.88
2-MMC : 4-MMC, 50:50_3	2-MMC (60%)	0.90	2-MMC (50%) + 4-MMC anhydrate (37%)	0.96	2-MMC (60%)	0.90
3-MMC : 4-MEC, 50:50_1	4-MEC (56%)	0.89	3-MMC (47%) + 4-MEC (42%)	0.98	2-MMC (48%) + Cellulose (8%)	0.78
3-MMC : 4-MEC, 50:50_2	4-MEC (55%)	0.90	3-MMC (48%) + 4-MEC (43%)	0.97	2-MMC (48%) + Cellulose (8%)	0.80
3-MMC : 4-MEC, 50:50_3	4-MEC (55%)	0.89	3-MMC (45%) + 4-MEC (45%)	0.97	4-MEC (55%)	0.88
3-MMC : 4-MEC, 75:25_1	3-MMC (64%)	0.91	3-MMC (70%) + 4-MEC (26%)	0.96	3-MMC (64%)	0.91
3-MMC : 4-MEC, 75:25_2	3-MMC (65%)	0.92	3-MMC (70%) + 4-MEC (27%)	0.97	3-MMC (64%)	0.92
3-MMC : 4-MEC, 75:25_3	3-MMC (65%)	0.92	3-MMC (71%) + 4-MEC (27%)	0.98	3-MMC (66%)	0.92
3-MMC : 4-MMC, 50:50_1	4-MMC anhydrate (63%)	0.92	3-MMC (46%) + 4-MMC anhydrate (42%)	0.97	4-MMC anhydrate (62%)	0.92
3-MMC : 4-MMC, 50:50_2	4-MMC anhydrate (63%)	0.92	3-MMC (46%) + 4-MMC anhydrate (44%)	0.97	4-MMC anhydrate (63%)	0.92
3-MMC : 4-MMC, 50:50_3	4-MMC anhydrate (65%)	0.93	3-MMC (44%) + 4-MMC anhydrate (45%)	0.96	4-MMC anhydrate (64%)	0.93
3-MMC : 4-MMC, 75:25_1	3-MMC (74%)	0.95	3-MMC (63%) + 4-MMC anhydrate (28%)	0.97	3-MMC (74%)	0.95
3-MMC : 4-MMC, 75:25_2	3-MMC (74%)	0.95	3-MMC (71%) + 4-MMC anhydrate (25%)	0.96	3-MMC (74%)	0.95
3-MMC : 4-MMC, 75:25_3	3-MMC (72%)	0.95	3-MMC (67%) + 4-MMC anhydrate (30%)	0.97	3-MMC (72%)	0.95
4-MMC : 4-MEC, 50:50_1	4-MEC (55%)	0.89	4-MEC (45%) + 4-MMC anhydrate (51%)	0.95	4-MEC (55%)	0.89
4-MMC : 4-MEC, 50:50_2	4-MEC (54%)	0.89	4-MEC (44%) + 4-MMC anhydrate (51%)	0.95	4-MEC (54%)	0.89
4-MMC : 4-MEC, 50:50_3	4-MEC (50%)	0.86	4-MEC (43%) + 4-MMC anhydrate (53%)	0.96	4-MEC (50%)	0.86

Note. The result in orange indicates that one of the two isomers is missed, results in gray on library options 1 and 3 are not relevant because they don't allow the detection of multiple drugs in a mixture. These are presented for information only.

Table S3. (part 1 of 2) Identification results of MMC/MEC containing casework samples in glass vials.

Code	Sample identity	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
D020_1	2-MMC	2-MMC (98%)	0.98	2-MMC (85%)	0.98	2-MMC (98%)	0.98
D020_2	2-MMC	2-MMC (98%)	0.98	2-MMC (98%)	0.98	2-MMC (98%)	0.98
D020_3	2-MMC	2-MMC (97%)	0.97	2-MMC (84%)	0.97	2-MMC (97%)	0.97
D022_1	3-MMC	3-MMC (96%)	0.96	3-MMC (96%)	0.96	3-MMC (85%)	0.96
D022_2	3-MMC	3-MMC (99%)	0.99	3-MMC (88%)	0.99	3-MMC (99%)	0.99
D022_3	3-MMC	3-MMC (97%)	0.97	3-MMC (83%)	0.97	3-MMC (97%)	0.97
MM001_1	3-MMC	3-MMC (61%)	0.90	3-MMC (61%)	0.90	3-MMC (60%)	0.90
MM001_2	3-MMC	3-MMC (59%)	0.93	3-MMC (58%)	0.93	3-MMC (58%)	0.93
MM001_3	3-MMC	3-MMC (59%)	0.92	3-MMC (56%)	0.92	3-MMC (59%)	0.92
MM002_1	3-MMC	3-MMC (60%)	0.91	3-MMC (58%)	0.91	3-MMC (61%)	0.91
MM002_2	3-MMC	3-MMC (56%)	0.89	3-MMC (51%)	0.89	3-MMC (54%)	0.89
MM002_3	3-MMC	3-MMC (60%)	0.91	3-MMC (61%)	0.91	3-MMC (61%)	0.91
MM003_1	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM003_2	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM003_3	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM004_1	3-MMC	3-MMC (72%)	0.97	3-MMC (72%)	0.97	3-MMC (72%)	0.97
MM004_2	3-MMC	3-MMC (96%)	0.96	3-MMC (76%)	0.96	3-MMC (76%)	0.96
MM004_3	3-MMC	3-MMC (94%)	0.94	3-MMC (70%)	0.94	3-MMC (94%)	0.94
MM005_1	3-MMC	3-MMC (97%)	0.97	3-MMC (97%)	0.97	3-MMC (97%)	0.97
MM005_2	3-MMC	3-MMC (97%)	0.97	3-MMC (97%)	0.97	3-MMC (97%)	0.97
MM005_3	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM006_1	4-MMC	4-MMC anhydrate (29%)	0.73	4-MMC hydrate (74%)	0.98	4-MMC hydrate (76%)	0.98
MM006_2	4-MMC	2-MMC (24%)	0.73	4-MMC hydrate (97%)	0.97	4-MMC hydrate (97%)	0.97
MM006_3	4-MMC	4-MEC (19%)	0.71	4-MMC hydrate (96%)	0.96	4-MMC hydrate (97%)	0.97
MM007_1	4-MMC (pink tablet, crushed)	4-MMC anhydrate (32%) + Cellulose (47%)	0.94	4-MMC anhydrate (16%) + 4-MMC hydrate (16%) + Cellulose (54%)	0.97	4-MMC hydrate (29%) + Cellulose (66%)	0.95
MM007_2	4-MMC (pink tablet, crushed)	4-MMC anhydrate (37%) + Cellulose (40%)	0.92	4-MMC anhydrate (22%) + 4-MMC hydrate (17%) + Cellulose (45%)	0.95	4-MMC anhydrate (37%) + Cellulose (40%)	0.92
MM007_3	4-MMC (pink tablet, crushed)	4-MMC anhydrate (33%) + Cellulose (47%)	0.94	4-MMC anhydrate (33%) + Cellulose (47%)	0.94	4-MMC anhydrate (33%) + Cellulose (47%)	0.94
MM008_1	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM008_2	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM008_3	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM009_1	3-MMC	3-MMC (98%)	0.98	3-MMC (85%)	0.98	3-MMC (98%)	0.98
MM009_2	3-MMC	3-MMC (98%)	0.98	3-MMC (88%)	0.98	3-MMC (98%)	0.98
MM009_3	3-MMC	3-MMC (83%)	0.98	3-MMC (83%)	0.98	3-MMC (84%)	0.98
MM010_1	3-MMC	3-MMC (96%)	0.96	3-MMC (96%)	0.96	3-MMC (96%)	0.96
MM010_2	3-MMC	3-MMC (97%)	0.97	3-MMC (97%)	0.97	3-MMC (97%)	0.97
MM010_3	3-MMC	3-MMC (97%)	0.97	3-MMC (97%)	0.97	3-MMC (97%)	0.97

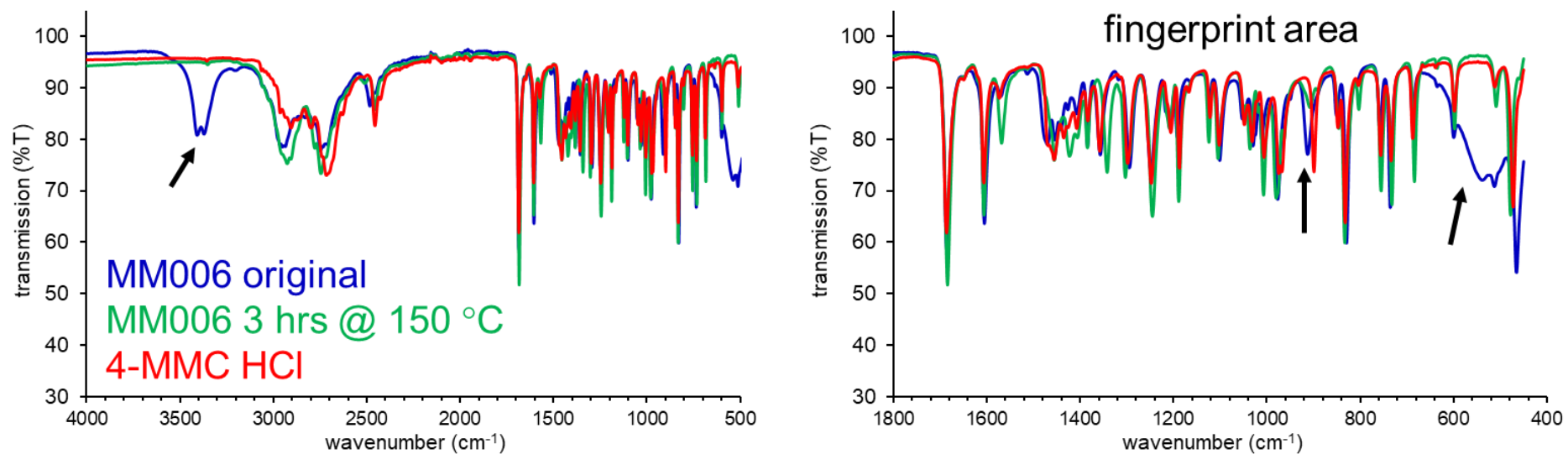
Note. Results in red indicate erroneous identifications, results in gray are below threshold and considered inconclusive. Results on library option 2 (multiple drug mixtures allowed) are presented for information only.

Table S3. (part 2 of 2) Identification results of MMC/MEC containing casework samples in glass vials.

Code	Sample identity	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
MM011_1	3-MMC	3-MMC (62%) + Cellulose (14%)	0.90	3-MMC (51%) + 2-MMC (23%)	0.88	3-MMC (61%) + Cellulose (14%)	0.89
MM011_2	3-MMC	3-MMC (64%) + Cellulose (13%)	0.90	3-MMC (53%)	0.88	3-MMC (64%) + Cellulose (13%)	0.90
MM011_3	3-MMC	3-MMC (57%)	0.89	3-MMC (59%)	0.89	3-MMC (60%)	0.89
MM012_1	3-MMC	3-MMC (52%)	0.88	3-MMC (52%)	0.88	3-MMC (51%)	0.88
MM012_2	3-MMC	3-MMC (56%)	0.91	3-MMC (57%)	0.91	3-MMC (57%)	0.90
MM012_3	3-MMC	3-MMC (51%)	0.88	3-MMC (52%)	0.88	3-MMC (52%)	0.88
MM013_1	3-MMC	3-MMC (97%)	0.97	3-MMC (97%)	0.97	3-MMC (97%)	0.97
MM013_2	3-MMC	3-MMC (99%)	0.99	3-MMC (99%)	0.99	3-MMC (99%)	0.99
MM013_3	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
MM014_1	4-MEC	4-MEC (78%)	0.96	4-MEC (78%)	0.97	4-MEC (97%)	0.97
MM014_2	4-MEC	4-MEC (97%)	0.97	4-MEC (97%)	0.97	4-MEC (97%)	0.97
MM014_3	4-MEC	4-MEC (75%)	0.96	4-MEC (74%)	0.96	4-MEC (75%)	0.96
MM015_1	4-MMC (blue tablet, crushed)	4-MMC anhydrate (54%) + Cellulose (29%)	0.94	4-MMC anhydrate (47%) + Cellulose (34%)	0.95	4-MMC anhydrate (54%) + Cellulose (29%)	0.94
MM015_2	4-MMC (blue tablet, crushed)	4-MMC anhydrate (53%) + Cellulose (32%)	0.96	4-MMC anhydrate (36%) + 2-MMC (18%) + Cellulose (31%)	0.96	4-MMC anhydrate (53%) + Cellulose (31%)	0.96
MM015_3	4-MMC (blue tablet, crushed)	4-MMC anhydrate (51%) + Cellulose (33%)	0.96	2-MMC (21%) + 4-MMC anhydrate (33%) + Cellulose (33%)	0.97	4-MMC anhydrate (51%) + Cellulose (33%)	0.96
MM016_1	4-MMC (brown tablet, crushed)	4-MMC anhydrate (42%) + Cellulose (42%)	0.96	4-MMC anhydrate (36%) + Cellulose (46%)	0.97	4-MMC anhydrate (42%) + Cellulose (42%)	0.96
MM016_2	4-MMC (brown tablet, crushed)	4-MMC anhydrate (41%) + Cellulose (41%)	0.95	4-MMC anhydrate (35%) + Cellulose (45%)	0.95	4-MMC anhydrate (41%) + Cellulose (40%)	0.95
MM016_3	4-MMC (brown tablet, crushed)	4-MMC anhydrate (38%) + Cellulose (44%)	0.95	4-MMC anhydrate (30%) + Cellulose (50%)	0.95	4-MMC anhydrate (38%) + Cellulose (44%)	0.95
MM017_1	4-MMC (green tablet, crushed)	4-MMC anhydrate (51%) + Cellulose (30%)	0.95	4-MMC anhydrate (52%) + Cellulose (30%)	0.95	4-MMC anhydrate (52%) + Cellulose (30%)	0.95
MM017_2	4-MMC (green tablet, crushed)	4-MMC anhydrate (46%) + Cellulose (35%)	0.95	4-MMC anhydrate (39%) + Cellulose (40%)	0.95	4-MMC anhydrate (46%) + Cellulose (35%)	0.95
MM017_3	4-MMC (green tablet, crushed)	4-MMC anhydrate (45%) + Cellulose (34%)	0.94	4-MMC anhydrate (39%) + Cellulose (40%)	0.94	4-MMC anhydrate (45%) + Cellulose (34%)	0.94
MM018_1	4-MMC	4-MMC anhydrate (24%)	0.71	4-MMC hydrate (99%)	0.99	4-MMC hydrate (99%)	0.99
MM018_2	4-MMC	4-MMC anhydrate (26%)	0.72	4-MMC hydrate (99%)	0.99	4-MMC hydrate (99%)	0.99
MM018_3	4-MMC	4-MEC (22%)	0.72	4-MMC hydrate (99%)	0.99	4-MMC hydrate (99%)	0.99
P102_1	4-MMC (orange tablet, crushed)	4-MMC anhydrate (55%) + Cellulose (31%)	0.96	4-MMC anhydrate (48%) + Cellulose (37%)	0.97	4-MMC anhydrate (54%) + Cellulose (31%)	0.96
P102_2	4-MMC (orange tablet, crushed)	4-MMC anhydrate (53%) + Cellulose (32%)	0.96	4-MMC anhydrate (45%) + Cellulose (38%)	0.96	4-MMC anhydrate (53%) + Cellulose (32%)	0.96
P102_3	4-MMC (orange tablet, crushed)	4-MMC anhydrate (48%) + Cellulose (34%)	0.95	4-MMC anhydrate (42%) + Cellulose (39%)	0.95	4-MMC anhydrate (48%) + Cellulose (34%)	0.95
PAM184_1	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
PAM184_2	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98
PAM184_3	3-MMC	3-MMC (98%)	0.98	3-MMC (98%)	0.98	3-MMC (98%)	0.98

Note. Results in red indicate erroneous identifications, results in gray are below threshold and considered inconclusive. Results on library option 2 (multiple drug mixtures allowed) are presented for information only.

Figure S5. FTIR spectra of 4-MMC HCl, case sample MM006, and case sample MM006 after heating.



Instrument: PerkinElmer (Waltham, MA) Spectrum Two FTIR with ATR option, scan range 400 to 1400 cm^{-1} .

Table S4. (part 1 of 3) Identification results of MMC/MEC containing casework samples in plastic bags.

Code	Sample identity	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
reference_1	2-MMC	2-MMC (71%) + Plastic LDPE bag (28%)	0.99	2-MMC (65%) + Plastic LDPE bag (27%)	0.99	2-MMC (71%) + Plastic LDPE bag (28%)	0.99
reference_2	2-MMC	2-MMC (73%) + Plastic LDPE bag (26%)	0.99	2-MMC (73%) + Plastic LDPE bag (26%)	0.99	2-MMC (73%) + Plastic LDPE bag (26%)	0.99
reference_3	2-MMC	2-MMC (65%) + Plastic LDPE bag (26%)	0.99	2-MMC (65%) + Plastic LDPE bag (26%)	0.99	2-MMC (65%) + Plastic LDPE bag (26%)	0.99
reference_1	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (68%) + Plastic LDPE bag (24%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
reference_2	3-MMC	3-MMC (70%) + Plastic LDPE bag (21%)	0.98	3-MMC (51%) + 2-MMC (21%)	0.87	3-MMC (69%) + Plastic LDPE bag (21%)	0.98
reference_3	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (73%) + Plastic LDPE bag (25%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
reference_1	4-MEC	4-MEC (70%) + Plastic LDPE bag (27%)	0.97	4-MEC (49%)	0.89	4-MEC (70%) + Plastic LDPE bag (27%)	0.97
reference_2	4-MEC	4-MEC (71%) + Plastic LDPE bag (27%)	0.97	4-MEC (49%)	0.89	4-MEC (71%) + Plastic LDPE bag (27%)	0.97
reference_3	4-MEC	4-MEC (70%) + Plastic LDPE bag (28%)	0.97	4-MEC (53%)	0.88	4-MEC (70%) + Plastic LDPE bag (27%)	0.97
reference_1	4-MMC	4-MMC Anhydrate (68%) + Plastic LDPE bag (24%)	0.99	4-MMC Anhydrate (68%) + Plastic LDPE bag (24%)	0.99	4-MMC Anhydrate (68%) + Plastic LDPE bag (24%)	0.99
reference_2	4-MMC	4-MMC Anhydrate (73%) + Plastic LDPE bag (26%)	0.99	4-MMC Anhydrate (73%) + Plastic LDPE bag (25%)	0.99	4-MMC Anhydrate (73%) + Plastic LDPE bag (26%)	0.99
reference_3	4-MMC	4-MMC Anhydrate (74%) + Plastic LDPE bag (24%)	0.98	4-MMC Anhydrate (74%) + Plastic LDPE bag (24%)	0.98	4-MMC Anhydrate (74%) + Plastic LDPE bag (24%)	0.98
blank_1	plastic bag	Plastic LDPE bag (99%)	0.99	Plastic LDPE bag (99%)	0.99	Plastic LDPE bag (99%)	0.99
blank_2	plastic bag	Plastic LDPE bag (99%)	0.99	Plastic LDPE bag (99%)	0.99	Plastic LDPE bag (99%)	0.99
blank_3	plastic bag	Plastic LDPE bag (100%)	1.00	Plastic LDPE bag (100%)	1.00	Plastic LDPE bag (100%)	1.00
D020_1	2-MMC	2-MMC (73%) + Plastic LDPE bag (26%)	0.99	2-MMC (73%) + Plastic LDPE bag (26%)	0.99	2-MMC (73%) + Plastic LDPE bag (26%)	0.99
D020_2	2-MMC	2-MMC (71%) + Plastic LDPE bag (26%)	0.98	2-MMC (71%) + Plastic LDPE bag (26%)	0.98	2-MMC (71%) + Plastic LDPE bag (26%)	0.97
D020_3	2-MMC	2-MMC (72%) + Plastic LDPE bag (26%)	0.98	2-MMC (72%) + Plastic LDPE bag (26%)	0.98	2-MMC (72%) + Plastic LDPE bag (26%)	0.98
D022_1	3-MMC	3-MMC (68%) + Plastic LDPE bag (23%)	0.99	3-MMC (68%) + Plastic LDPE bag (23%)	0.99	3-MMC (68%) + Plastic LDPE bag (23%)	0.99
D022_2	3-MMC	3-MMC (69%) + Plastic LDPE bag (23%)	0.99	3-MMC (52%)	0.85	3-MMC (69%) + Plastic LDPE bag (23%)	0.99
D022_3	3-MMC	3-MMC (68%) + Plastic LDPE bag (23%)	0.99	3-MMC (54%)	0.85	3-MMC (73%) + Plastic LDPE bag (26%)	0.99
MM001_1	3-MMC	3-MMC (53%) + Plastic LDPE bag (30%)	0.96	3-MMC (53%) + Plastic LDPE bag (30%)	0.96	3-MMC (53%) + Plastic LDPE bag (30%)	0.96
MM001_2	3-MMC	3-MMC (54%) + Plastic LDPE bag (29%)	0.97	3-MMC (54%) + Plastic LDPE bag (29%)	0.97	3-MMC (54%) + Plastic LDPE bag (29%)	0.97
MM001_3	3-MMC	3-MMC (45%) + Plastic LDPE bag (34%)	0.95	3-MMC (28%) + 2-MMC (34%) + Plastic LDPE bag (34%)	0.96	3-MMC (45%) + Plastic LDPE bag (34%)	0.95
MM002_1	3-MMC	3-MMC (56%) + Plastic LDPE bag (31%)	0.98	3-MMC (42%) + 2-MMC (21%) + Plastic LDPE bag (27%)	0.98	3-MMC (56%) + Plastic LDPE bag (31%)	0.98
MM002_2	3-MMC	3-MMC (58%) + Plastic LDPE bag (29%)	0.98	3-MMC (58%) + Plastic LDPE bag (29%)	0.98	3-MMC (58%) + Plastic LDPE bag (29%)	0.98
MM002_3	3-MMC	3-MMC (64%) + Plastic LDPE bag (32%)	0.96	3-MMC (64%) + Plastic LDPE bag (32%)	0.95	3-MMC (64%) + Plastic LDPE bag (32%)	0.96
MM003_1	3-MMC	3-MMC (69%) + Plastic LDPE bag (30%)	0.99	3-MMC (69%) + Plastic LDPE bag (30%)	0.99	3-MMC (69%) + Plastic LDPE bag (30%)	0.99
MM003_2	3-MMC	3-MMC (68%) + Plastic LDPE bag (31%)	0.99	3-MMC (68%) + Plastic LDPE bag (31%)	0.99	3-MMC (68%) + Plastic LDPE bag (31%)	0.99
MM003_3	3-MMC	3-MMC (70%) + Plastic LDPE bag (29%)	0.98	3-MMC (70%) + Plastic LDPE bag (29%)	0.98	3-MMC (70%) + Plastic LDPE bag (29%)	0.98
MM004_1	3-MMC	3-MMC (47%)	0.86	3-MMC (48%)	0.86	3-MMC (48%)	0.86
MM004_2	3-MMC	3-MMC (74%) + Plastic LDPE bag (18%)	0.92	3-MMC (61%) + Plastic LDPE bag (16%)	0.92	3-MMC (74%) + Plastic LDPE bag (18%)	0.92
MM004_3	3-MMC	3-MMC (51%)	0.88	3-MMC (51%)	0.87	3-MMC (51%)	0.87
MM005_1	3-MMC	3-MMC (68%) + Plastic LDPE bag (20%)	0.98	3-MMC (69%) + Plastic LDPE bag (20%)	0.98	3-MMC (68%) + Plastic LDPE bag (20%)	0.98
MM005_2	3-MMC	3-MMC (78%) + Plastic LDPE bag (21%)	0.99	3-MMC (78%) + Plastic LDPE bag (21%)	0.99	3-MMC (78%) + Plastic LDPE bag (21%)	0.99
MM005_3	3-MMC	3-MMC (68%) + Plastic LDPE bag (17%)	0.97	3-MMC (68%) + Plastic LDPE bag (17%)	0.97	3-MMC (77%) + Plastic LDPE bag (20%)	0.97

Note. Results in **red** indicate erroneous identifications. Library options 1 (only 4-MMC anhydrate) and 2 (multiple drug mixtures allowed) are presented for information only. Results from library option 3 in **gray** are indicative only due to the 0.80 similarity score threshold.

Table S4. (part 2 of 3) Identification results of MMC/MEC containing casework samples in plastic bags.

Code	Sample identity	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
MM006_1	4-MMC	2-MMC (48%) + Plastic LDPE bag (16%)	0.85	4-MMC Hydrate (66%) + Plastic LDPE bag (33%)	0.99	4-MMC Hydrate (62%) + Plastic LDPE bag (30%)	0.99
MM006_2	4-MMC	2-MMC (48%) + Plastic LDPE bag (14%)	0.84	4-MMC Hydrate (61%) + Plastic LDPE bag (28%)	0.99	4-MMC Hydrate (62%) + Plastic LDPE bag (28%)	0.99
MM006_3	4-MMC	2-MMC (47%) + Plastic LDPE bag (13%)	0.83	4-MMC Hydrate (62%) + Plastic LDPE bag (27%)	0.99	4-MMC Hydrate (62%) + Plastic LDPE bag (27%)	0.99
MM007_1	4-MMC (pink tablet, crushed)	4-MEC (25%) + Plastic LDPE bag (35%)	0.78	4-MEC (25%) + Plastic LDPE bag (34%)	0.78	4-MEC (25%) + Plastic LDPE bag (34%)	0.78
MM007_2	4-MMC (pink tablet, crushed)	4-MMC Anhydrate (28%) + Plastic LDPE bag (29%)	0.75	4-MEC (25%) + Plastic LDPE bag (30%)	0.74	4-MMC Anhydrate (28%) + Plastic LDPE bag (29%)	0.75
MM007_3	4-MMC (pink tablet, crushed)	4-MMC Anhydrate (30%) + Plastic LDPE bag (32%)	0.78	4-MMC Anhydrate (30%) + Plastic LDPE bag (31%)	0.78	4-MMC Anhydrate (29%) + Plastic LDPE bag (32%)	0.78
MM008_1	3-MMC	3-MMC (69%) + Plastic LDPE bag (30%)	0.99	3-MMC (69%) + Plastic LDPE bag (30%)	0.99	3-MMC (69%) + Plastic LDPE bag (30%)	0.99
MM008_2	3-MMC	3-MMC (72%) + Plastic LDPE bag (27%)	0.99	3-MMC (72%) + Plastic LDPE bag (27%)	0.99	3-MMC (72%) + Plastic LDPE bag (27%)	0.99
MM008_3	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (55%)	0.86	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
MM009_1	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
MM009_2	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
MM009_3	3-MMC	3-MMC (72%) + Plastic LDPE bag (26%)	0.99	3-MMC (72%) + Plastic LDPE bag (26%)	0.99	3-MMC (72%) + Plastic LDPE bag (26%)	0.99
MM010_1	3-MMC	3-MMC (68%) + Plastic LDPE bag (24%)	0.99	3-MMC (47%)	0.85	3-MMC (68%) + Plastic LDPE bag (24%)	0.99
MM010_2	3-MMC	3-MMC (74%) + Plastic LDPE bag (25%)	0.99	3-MMC (56%)	0.86	3-MMC (74%) + Plastic LDPE bag (25%)	0.99
MM010_3	3-MMC	3-MMC (73%) + Plastic LDPE bag (26%)	0.99	3-MMC (73%) + Plastic LDPE bag (26%)	0.99	3-MMC (73%) + Plastic LDPE bag (26%)	0.99
MM011_1	3-MMC	3-MMC (53%) + Plastic LDPE bag (27%)	0.94	3-MMC (35%) + 2-MMC (25%) + Plastic LDPE bag (24%)	0.95	3-MMC (53%) + Plastic LDPE bag (27%)	0.94
MM011_2	3-MMC	3-MMC (55%) + Plastic LDPE bag (27%)	0.95	3-MMC (41%) + 2-MMC (28%) + Plastic LDPE bag (26%)	0.96	3-MMC (54%) + Plastic LDPE bag (27%)	0.95
MM011_3	3-MMC	2-MMC (59%) + Plastic LDPE bag (19%)	0.93	3-MMC (38%) + 2-MMC (27%) + Plastic LDPE bag (21%)	0.97	3-MMC (57%) + Plastic LDPE bag (25%)	0.95
MM012_1	3-MMC	3-MMC (52%) + Plastic LDPE bag (31%)	0.96	3-MMC (33%) + 2-MMC (27%) + Plastic LDPE bag (27%)	0.97	3-MMC (52%) + Plastic LDPE bag (31%)	0.96
MM012_2	3-MMC	3-MMC (54%) + Plastic LDPE bag (30%)	0.97	3-MMC (33%) + 2-MMC (28%) + Plastic LDPE bag (26%)	0.98	3-MMC (54%) + Plastic LDPE bag (30%)	0.97
MM012_3	3-MMC	3-MMC (54%) + Plastic LDPE bag (30%)	0.97	3-MMC (34%) + 2-MMC (27%) + Plastic LDPE bag (26%)	0.97	3-MMC (54%) + Plastic LDPE bag (30%)	0.97
MM013_1	3-MMC	3-MMC (67%) + Plastic LDPE bag (25%)	0.99	3-MMC (67%) + Plastic LDPE bag (25%)	0.99	3-MMC (67%) + Plastic LDPE bag (25%)	0.99
MM013_2	3-MMC	3-MMC (71%) + Plastic LDPE bag (28%)	0.99	3-MMC (52%)	0.85	3-MMC (71%) + Plastic LDPE bag (28%)	0.99
MM013_3	3-MMC	3-MMC (71%) + Plastic LDPE bag (28%)	0.99	3-MMC (71%) + Plastic LDPE bag (28%)	0.99	3-MMC (71%) + Plastic LDPE bag (28%)	0.99
MM014_1	4-MEC	4-MEC (58%) + Plastic LDPE bag (25%)	0.95	4-MEC (58%) + Plastic LDPE bag (25%)	0.95	4-MEC (58%) + Plastic LDPE bag (25%)	0.95
MM014_2	4-MEC	4-MEC (59%) + Plastic LDPE bag (25%)	0.95	4-MEC (59%) + Plastic LDPE bag (25%)	0.95	4-MEC (59%) + Plastic LDPE bag (25%)	0.95
MM014_3	4-MEC	4-MEC (61%) + Plastic LDPE bag (25%)	0.96	4-MEC (61%) + Plastic LDPE bag (25%)	0.96	4-MEC (68%) + Plastic LDPE bag (28%)	0.96
MM015_1	4-MMC (blue tablet, crushed)	4-MMC Anhydrate (42%) + Plastic LDPE bag (29%)	0.85	4-MMC Anhydrate (42%) + Plastic LDPE bag (29%)	0.85	4-MMC Anhydrate (42%) + Plastic LDPE bag (29%)	0.85
MM015_2	4-MMC (blue tablet, crushed)	4-MMC Anhydrate (43%) + Plastic LDPE bag (28%)	0.84	4-MMC Anhydrate (43%) + Plastic LDPE bag (27%)	0.84	4-MMC Anhydrate (43%) + Plastic LDPE bag (27%)	0.84
MM015_3	4-MMC (blue tablet, crushed)	4-MMC Anhydrate (42%) + Plastic LDPE bag (27%)	0.84	4-MMC Anhydrate (41%) + Plastic LDPE bag (26%)	0.84	4-MMC Anhydrate (41%) + Plastic LDPE bag (26%)	0.83
MM016_1	4-MMC (brown tablet, crushed)	4-MMC Anhydrate (32%) + Plastic LDPE bag (27%)	0.77	4-MMC Anhydrate (33%) + Plastic LDPE bag (27%)	0.77	4-MMC Anhydrate (33%) + Plastic LDPE bag (27%)	0.77
MM016_2	4-MMC (brown tablet, crushed)	4-MMC Anhydrate (32%) + Plastic LDPE bag (26%)	0.77	4-MMC Anhydrate (29%) + Plastic LDPE bag (30%)	0.76	4-MMC Anhydrate (33%) + Plastic LDPE bag (27%)	0.77
MM016_3	4-MMC (brown tablet, crushed)	4-MMC Anhydrate (32%) + Plastic LDPE bag (25%)	0.75	4-MMC Anhydrate (33%) + Plastic LDPE bag (25%)	0.76	4-MMC Anhydrate (32%) + Plastic LDPE bag (25%)	0.76
MM017_1	4-MMC (green tablet, crushed)	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (36%) + Plastic LDPE bag (31%)	0.82	4-MMC Anhydrate (39%) + Plastic LDPE bag (28%)	0.83
MM017_2	4-MMC (green tablet, crushed)	4-MMC Anhydrate (39%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (39%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (39%) + Plastic LDPE bag (28%)	0.82
MM017_3	4-MMC (green tablet, crushed)	4-MMC Anhydrate (39%) + Plastic LDPE bag (29%)	0.83	4-MMC Anhydrate (39%) + Plastic LDPE bag (29%)	0.83	4-MMC Anhydrate (39%) + Plastic LDPE bag (29%)	0.83

Note. Results in red indicate erroneous identifications. Library options 1 (only 4-MMC anhydrate) and 2 (multiple drug mixtures allowed) are presented for information only. Results from library option 3 in gray are indicative only due to the 0.80 similarity score threshold.

Table S4. (part 3 of 3) Identification results of MMC/MEC containing casework samples in plastic bags.

Code	Sample identity	Model result (library option 1)	Similarity	Model result (library option 2)	Similarity	Model result (library option 3)	Similarity
MM018_1	4-MMC	2-MMC (47%) + Plastic LDPE bag (17%)	0.85	4-MMC Hydrate (69%) + Plastic LDPE bag (31%)	0.99	4-MMC Hydrate (69%) + Plastic LDPE bag (31%)	0.99
MM018_2	4-MMC	2-MMC (47%) + Plastic LDPE bag (17%)	0.84	4-MMC Hydrate (68%) + Plastic LDPE bag (31%)	0.99	4-MMC Hydrate (69%) + Plastic LDPE bag (31%)	0.99
MM018_3	4-MMC	2-MMC (47%) + Plastic LDPE bag (17%)	0.85	4-MMC Hydrate (65%) + Plastic LDPE bag (30%)	0.99	4-MMC Hydrate (65%) + Plastic LDPE bag (30%)	0.99
P102_1	4-MMC (orange tablet, crushed)	4-MMC Anhydrate (40%) + Plastic LDPE bag (27%)	0.83	4-MMC Anhydrate (40%) + Plastic LDPE bag (27%)	0.83	4-MMC Anhydrate (40%) + Plastic LDPE bag (27%)	0.83
P102_2	4-MMC (orange tablet, crushed)	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83
P102_3	4-MMC (orange tablet, crushed)	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83	4-MMC Anhydrate (40%) + Plastic LDPE bag (29%)	0.84	4-MMC Anhydrate (40%) + Plastic LDPE bag (28%)	0.83
PAM184_1	3-MMC	3-MMC (76%) + Plastic LDPE bag (22%)	0.98	3-MMC (76%) + Plastic LDPE bag (22%)	0.98	3-MMC (76%) + Plastic LDPE bag (22%)	0.98
PAM184_2	3-MMC	3-MMC (69%) + Plastic LDPE bag (20%)	0.98	3-MMC (69%) + Plastic LDPE bag (20%)	0.98	3-MMC (70%) + Plastic LDPE bag (20%)	0.98
PAM184_3	3-MMC	3-MMC (68%) + Plastic LDPE bag (20%)	0.98	3-MMC (76%) + Plastic LDPE bag (22%)	0.98	3-MMC (75%) + Plastic LDPE bag (22%)	0.98

Note. Results in red indicate erroneous identifications. Library options 1 (only 4-MMC anhydrate) and 2 (multiple drug mixtures allowed) are presented for information only. Results from library option 3 in gray are indicative only due to the 0.80 similarity score threshold.