Supplementary Information

A Validated NMR Approach for MDMA Quantification in Ecstasy Tablets

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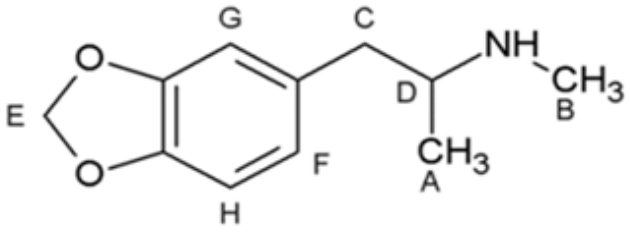
Table S1. ^{1}H NMR chemical shifts, multiplicity, integral and coupling constant for MDMA.HCl in D_2O



Hydrogens identification	Chemical shift / ppm	Multiplicity	Integral	Coupling constant (*J*) / Hz
H_A	1.27	doublet	3	6.6
H_B	2.70	singlet	3	–
H_{C1}	2.83	doublet of doublets	1	7.9/14.1
H_{C2}	2.97	doublet of doublets	1	6.6/14.1
H_D	3.48	multiplet	1	–
H_E	5.97	singlet	2	–
H_F	6.78	doublet of doublets	1	1.8 / 7.9
H_G	6.84	doublet	1	1.8
H_H	6.88	doublet	1	7.9

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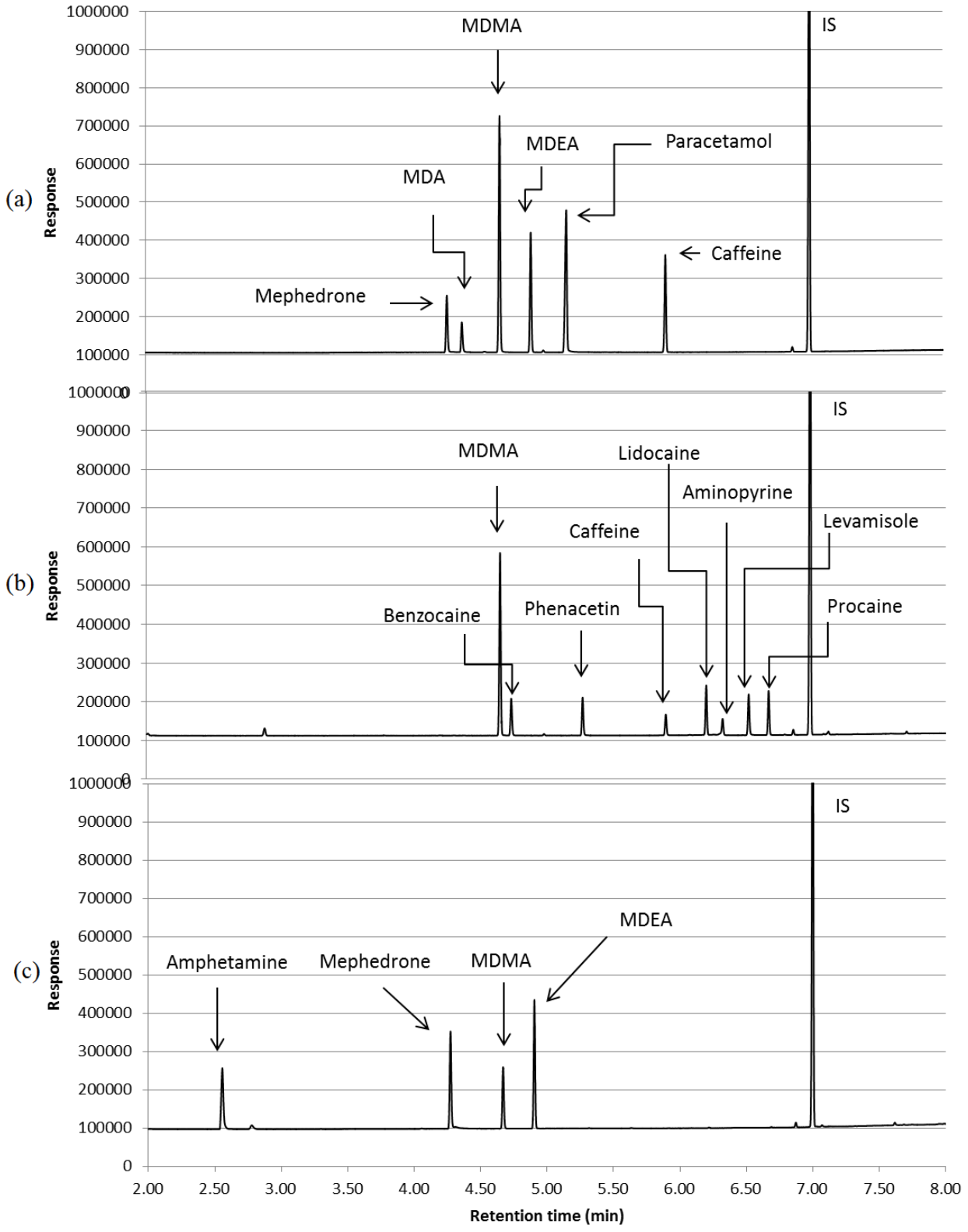

Figure S1. GC-FID chromatograms of different mixtures of internal standard (IS), MDMA and adulterants in ecstasy tablets. (a) Caffeine, paracetamol, MDEA, MDMA and mephedrone; (b) procaine, levamisole, aminopyrine, lidocaine, caffeine, phenacetin and benzocaine; (c) MDEA, mephedrone and amphetamine.

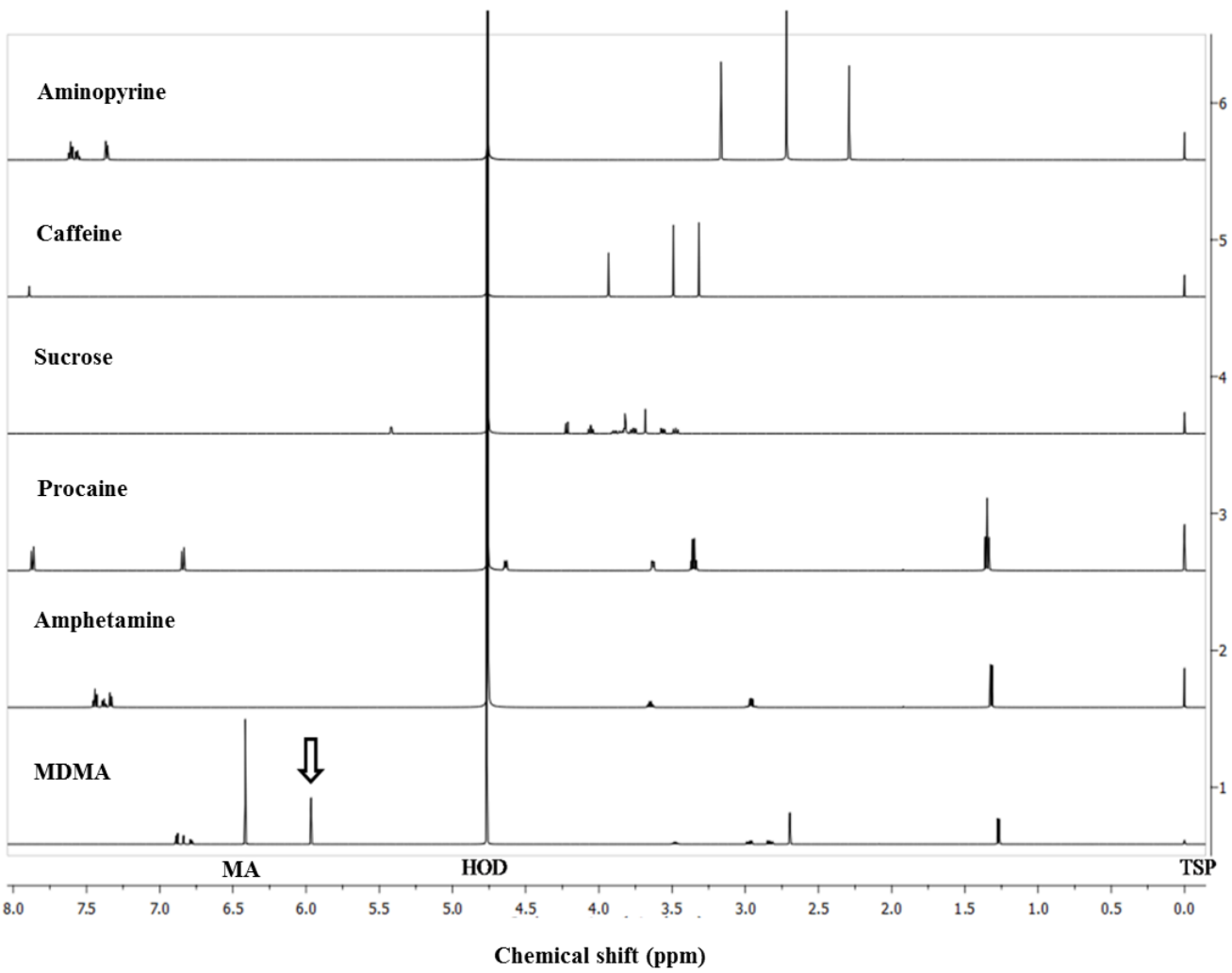

Figure S2. ^{1}H NMR spectra (600.13 MHz, D_2O) of different contaminants of ecstasy tablets: aminopyrine; caffeine; sucrose; procaine and amphetamine and MDMA and MA. Arrow indicates MDMA signal used in quantification analyses.