

Supporting Information

Analyses of Drugs of Abuse in Biofluids and Solid Matrices by Low Temperature Plasma (LTP) Ionization Mass Spectrometry

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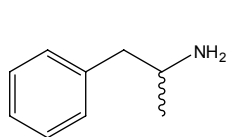
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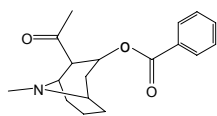
Abstract: The structures of the analytes as well as details of the referenced liquid chromatography method used to confirm the LTP-MS/MS analysis of real samples is provided. The decay profile of the caffeine metabolism is provided. Results of the LC-MS confirmation for the detection of cocaine within a hair extract are presented.

Liquid Chromatography Electrospray Mass Spectrometry Reference Method

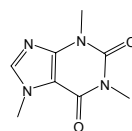
A Zorbax HT XDB-C₁₈ analytical column of the following dimensions: 4.6 mm x 50 mm and 1.8 µm particle size (Agilent Technologies) was used in the HPLC analysis. The mobile phases used were water with 0.1% formic acid (A) and acetonitrile (B). The chromatographic method held the initial mobile phase composition (10% B) constant for 3 min, followed by a linear gradient to 100% B up to 15 min and kept for 5 min at 100% B. The flow rate used was 0.5 mLmin⁻¹. The HPLC system was connected to a time-of-flight mass spectrometer (Agilent 6220 accurate mass TOF, Agilent Technologies, Santa Clara, CA, USA) equipped with an electrospray interface operating in positive ion mode using the following operating parameters: capillary voltage 4000 V; nebulizer pressure 40 psig; drying gas flow rate 9.0 L min⁻¹; gas temperature 325° C; skimmer voltage 65 V; octapole 1 rf 250 V; fragmenter voltage 190 V. LC-MS accurate mass spectra were recorded across the range of m/z 50-1000.



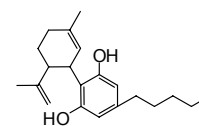
Amphetamine
mw 135 g/mol



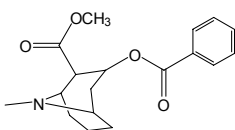
Benzoylcegonine
mw 290 g/mol



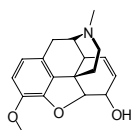
Caffeine
mw 194 g/mol



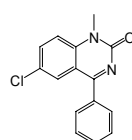
Cannabidiol
mw 314 g/mol



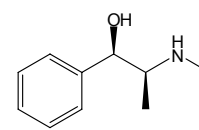
Cocaine
mw 303 g/mol



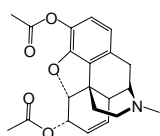
Codeine
mw 299 g/mol



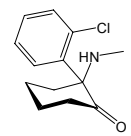
Diazepam
mw 284 g/mol



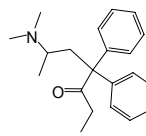
Ephedrine
mw 165 g/mol



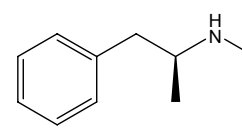
Heroin
mw 369 g/mol



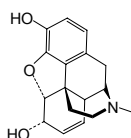
Ketamine
mw 237 g/mol



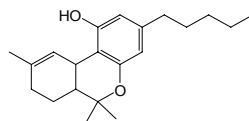
Methadone
mw 309 g/mol



Methamphetamine
mw 149 g/mol



Morphine
mw 285 g/mol



Δ9 – THC
mw 314 g/mol

Figure S1. Structure and nominal mass of drugs of abuse

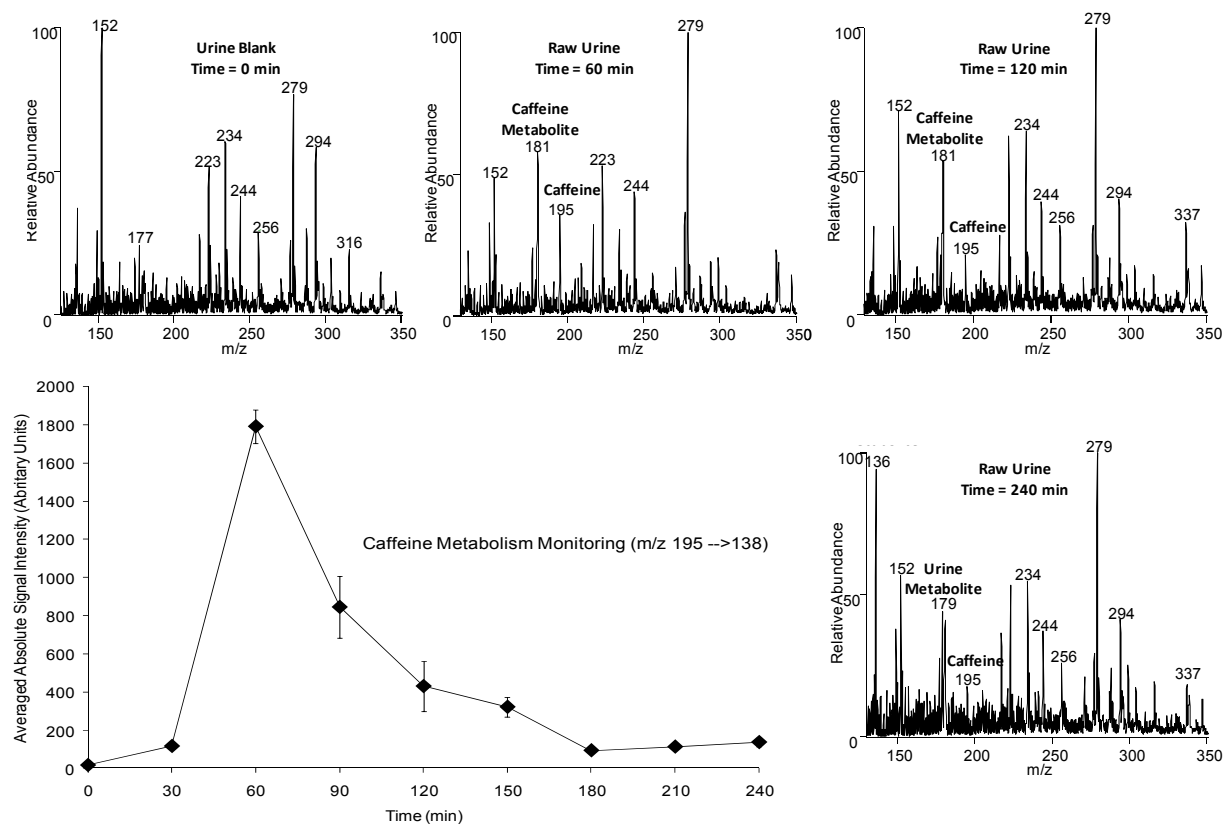


Figure S2. Direct monitoring of caffeine (m/z 195) in raw urine after consumption of a caffeinated drink. The full mass spectra (m/z 125 – 350) at different time points in the decay profile are presented. The decay profile is a generated based on the LTP-MS/MS monitoring of caffeine's major fragment ion (m/z 195 \rightarrow 138).

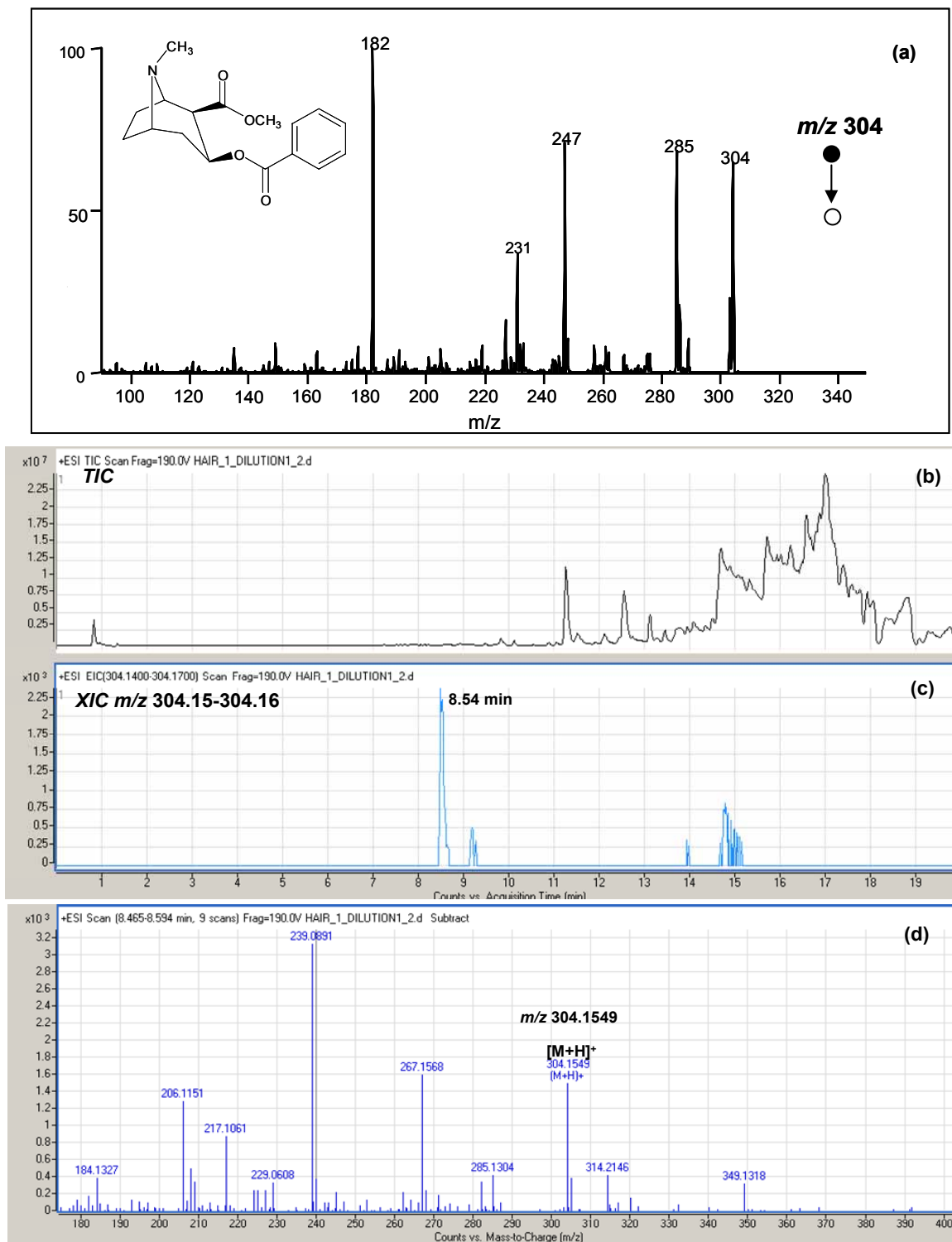


Figure S3. a) LTP-MS/MS detection of cocaine (m/z 304 \rightarrow 182) in a hair extract containing 1.4 pg by LC-MS analysis; b) total ion chromatogram obtained from the LC-TOFMS analysis of the studied hair extract; c) extracted ion chromatogram (m/z 304.15 – 304.16); the retention time of cocaine is 8.50 min; d) Accurate mass spectrum at 8.50 min. The experimental spectrum shows a peak with m/z 304.1549 (theoretical mass spectrum of cocaine: 304.1543)