

Supporting information

Isomer-Specific Two-Color Double-Resonance IR²MS³ Ion Spectroscopy using a Single Laser: Application in the Identification of Novel Psychoactive Substances

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Table S1. GC-MS experimental details

Instrument:	Agilent Technologies 7890B GC with 5977B single quadrupole mass spectrometer
GC method:	1 μ L injection split injection (1:68) @ 300 °C column: 30 m HP-5MS, 0.25 mm internal diameter, 0.25 μ m film thickness oven: start at 100 °C, 1.5 min hold time, ramp at 30 °C/min to 300 °C
MS method:	transfer line: 280 °C; MS source temperature: 230 °C; quadrupole temperature: 150 °C ionization mode: 70 eV electron ionization acquisition mode: full scan from m/z 41 to m/z 462 with scan speed 3.125 scans/sec.
MS library search:	mass spectra from a chromatographic peak were averaged and baseline subtracted resulting peak spectrum was searched in NIST MS Search version 2.3. MS match scores were returned on a 0 to 1000 scale

Table S2. MS library match scores above 900 for peaks A and B in the GC-MS chromatogram of the case sample shown in Figure 1. sw = SWGDRUG 3.3 spectral library, M = NIST14 main library, R = NIST14 replicate library, ca = Cayman Spectral Library version 12212018, match = forward search match score, r.match = reversed search match score.

library	match	r.match	name (peak A; 3.703 min.)
sw	919	919	2-fluoromethamphptamine
M	919	919	4-fluoromethamphetamine
M	919	919	2-fluoromethamphetamine
sw	917	920	4-fluoromethamphetamine
R	917	920	4-fluoromethamphetamine
ca	911	923	4-fluoromethamphetamine
M	911	923	4-fluoromethamphetamine
sw	903	913	3-fluoromethamphetamine
library	match	r.match	name (peak B; 3.737 min.)
sw	959	959	4-fluoromethamphetamine
R	959	959	4-fluoromethamphetamine
M	956	956	4-fluoromethamphetamine
sw	937	937	2-fluoromethamphptamine
M	937	937	2-fluoromethamphptamine
ca	931	944	4-fluoromethamphetamine
M	931	944	4-fluoromethamphetamine
sw	927	940	3-fluoromethamphetamine
ca	917	929	3-fluoromethamphetamine