

1. GENERAL INFORMATION

IUPAC Name:	(2-iodophenyl)[1-(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]methanone
CFR:	Not Scheduled (02/2013)
CAS #:	444912-75-8
Synonyms:	1-[(N-methylpiperidin-2-yl)methyl]-3-(2-iodobenzoyl)indole
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UV_{max}(nm):	Not Available

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₂ H ₂₃ IN ₂ O	458	144.9

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

N. Uchiyama, M. Kawamura, R. Kikura-Hanajiri, Y. Goda. Identification of two new-type synthetic cannabinoids, *N*-(1-adamantyl)-1-pentyl-1*H*-indole-3-carboxamide (APICA) and *N*-(1-adamantyl)-1-pentyl-1*H*-indazole-3-carboxamide (APINACA), and detection of five synthetic cannabinoids, AM-1220, AM-2233, AM-1241, CB-13 (CRA-13), AND AM-1248, as designer drugs in illegal products. *Forensic Toxicology* 2012; 30(2): 114-125.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

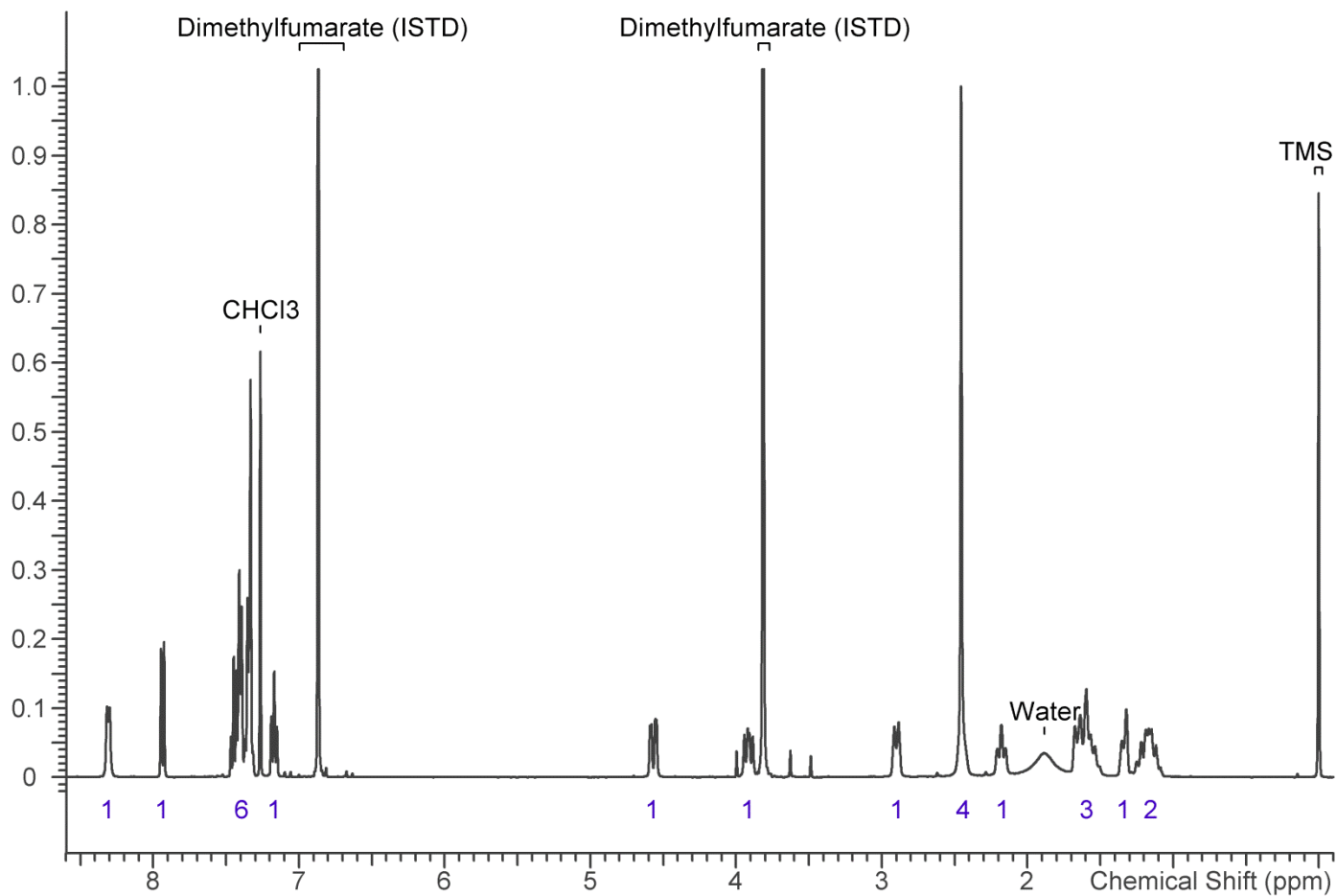
Sample Preparation: Dilute analyte to ~5mg/mL in deuteriochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

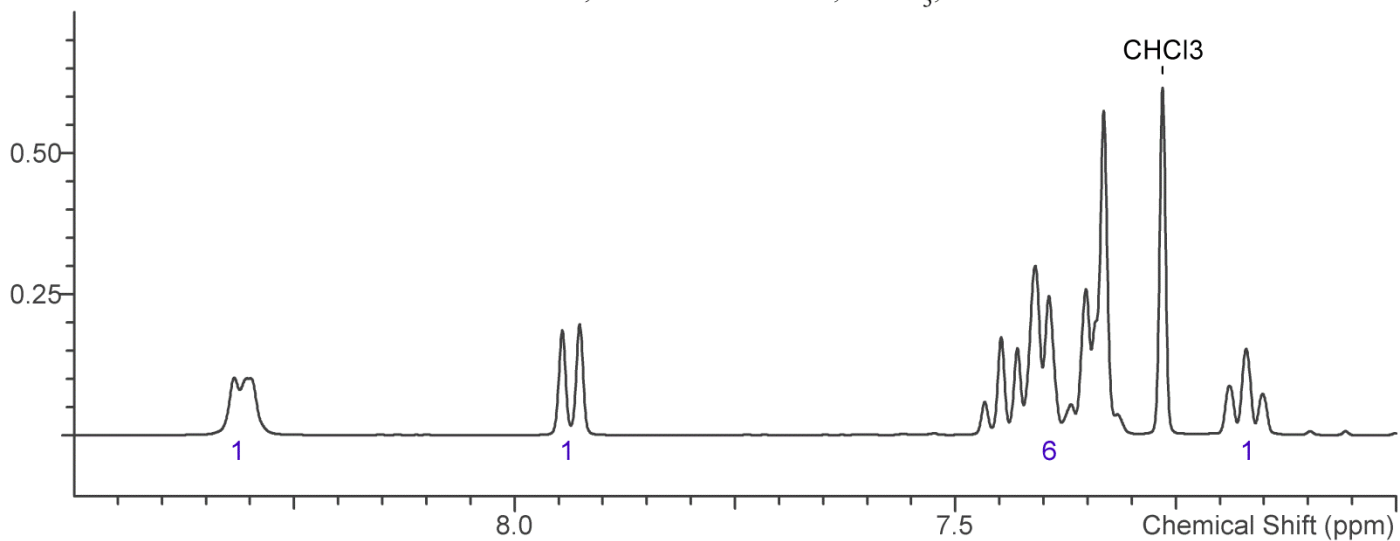
Parameters:

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

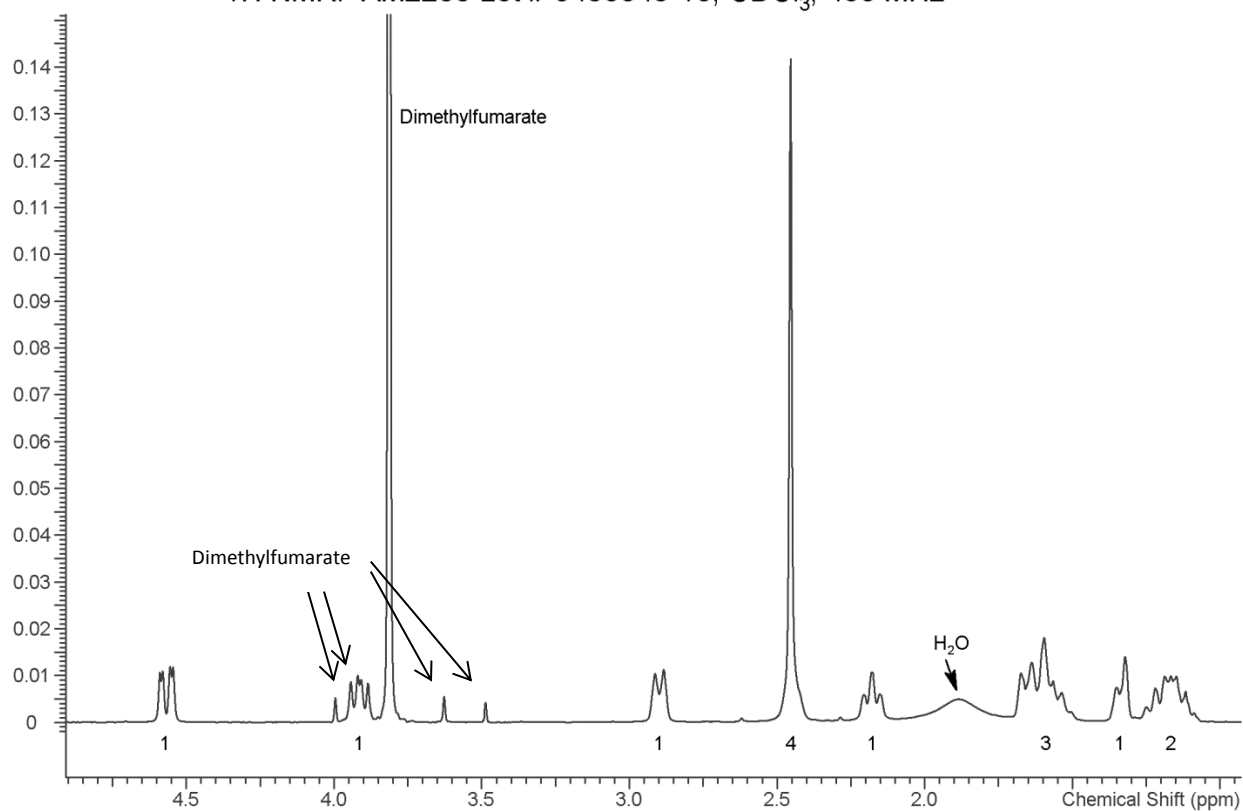
^1H NMR: AM2233; Lot # 0436043-18, CDCl_3 , 400 MHz



^1H NMR: AM2233; Lot # 0436043-18, CDCl_3 , 400 MHz



1H NMR: AM2233 Lot # 0436043-18, CDCl₃, 400 MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in MeOH.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS; 30m x .25mm x .25 μ m

Carrier Gas: Helium at 1 mL/min

Temperatures:
Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C

Oven program:

1) 100°C initial temperature for 1.0 min

2) Ramp to 300°C at 12°C/min

3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 30-550 amu

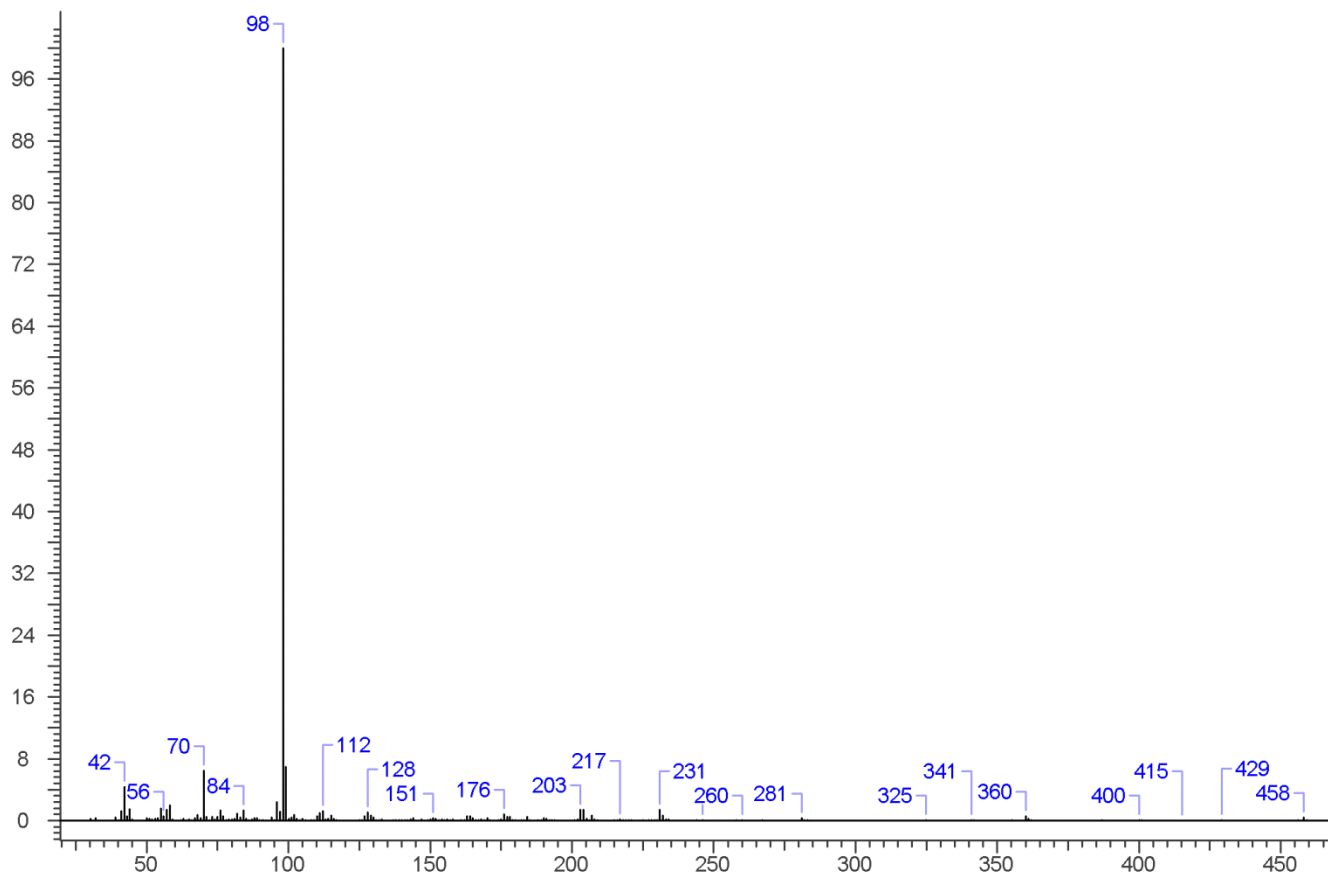
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 22.019 minutes

El Mass Spectrum: AM2233 Lot # 0436043-18



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument:

FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:

Number of scans: 32

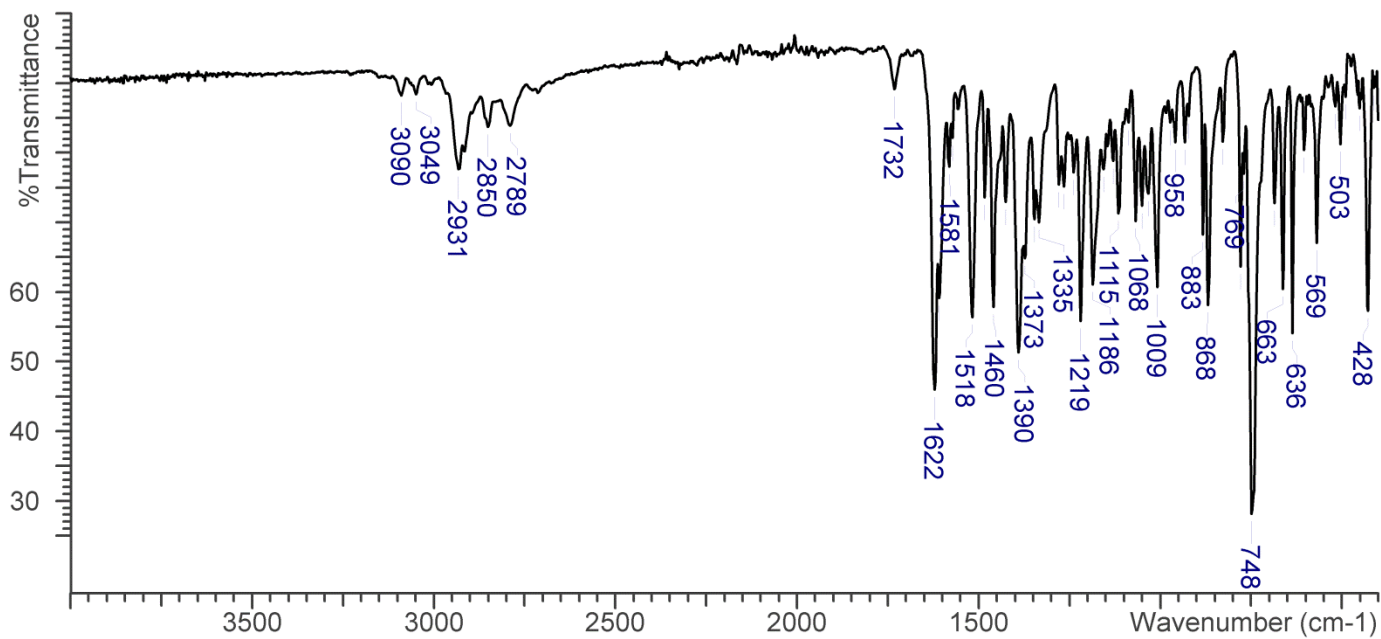
Number of background scans: 32

Resolution: 4cm^{-1}

Sample gain: 8

Aperture: 150

FTIR ATR (Diamond, 3 Bounce): AM2233 Lot # 0436043-18



FTIR ATR (Diamond, 3 Bounce): AM2233 Lot # 0436043-18

