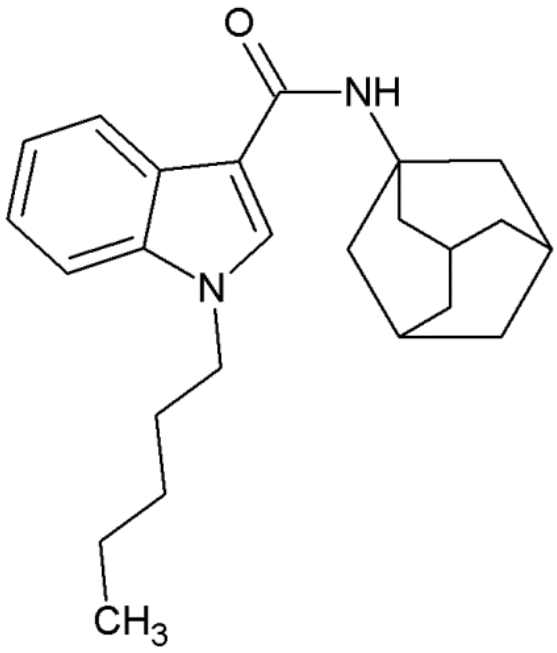


1. GENERAL INFORMATION

IUPAC Name: 1-pentyl-N-(tricyclo[3.3.1.1 ^{3,7}]dec-1-yl)-1H-indole-3 carboxamide

CFR: Not Scheduled (03/2013)

CAS #: 1345973-50-3

Synonyms: 2NE1, APICA

Source: DEA Reference Material Collection

Appearance: White powder

Kovat's Index: Pending

UV_{max}: Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{24}H_{32}N_2O$	364	141.6

3. ADDITIONAL RESOURCES

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.

Forendex

Wikipedia

4. QUALITATIVE DATA

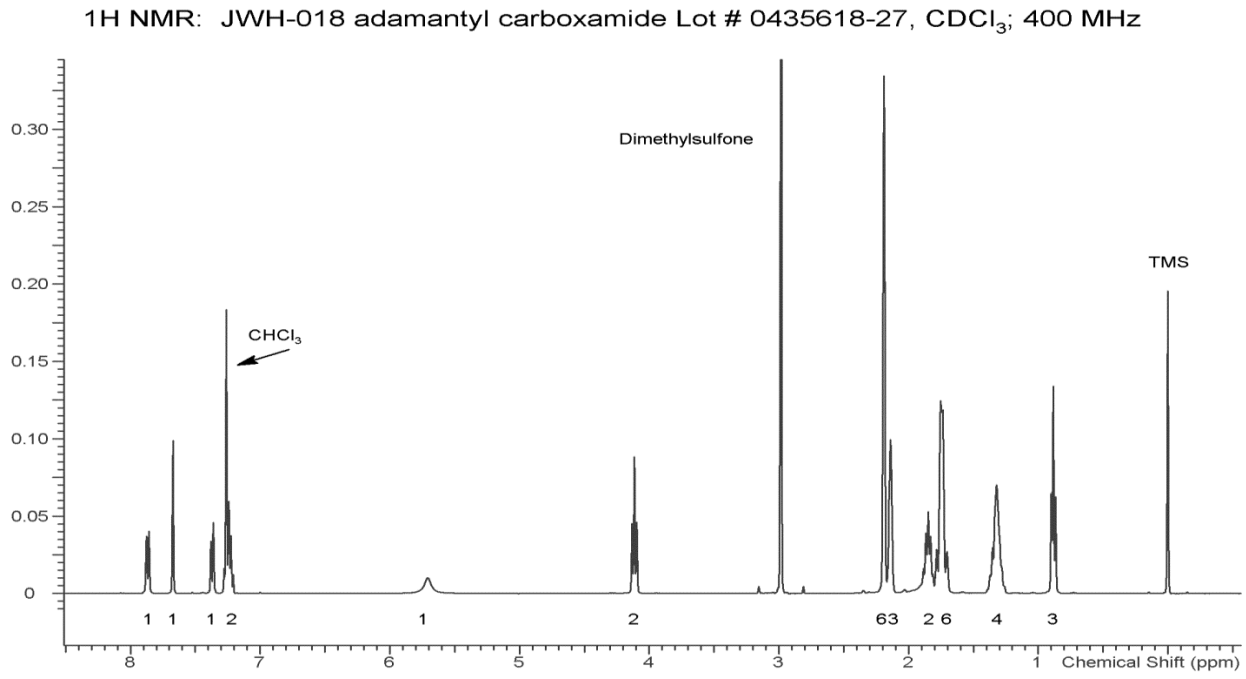
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

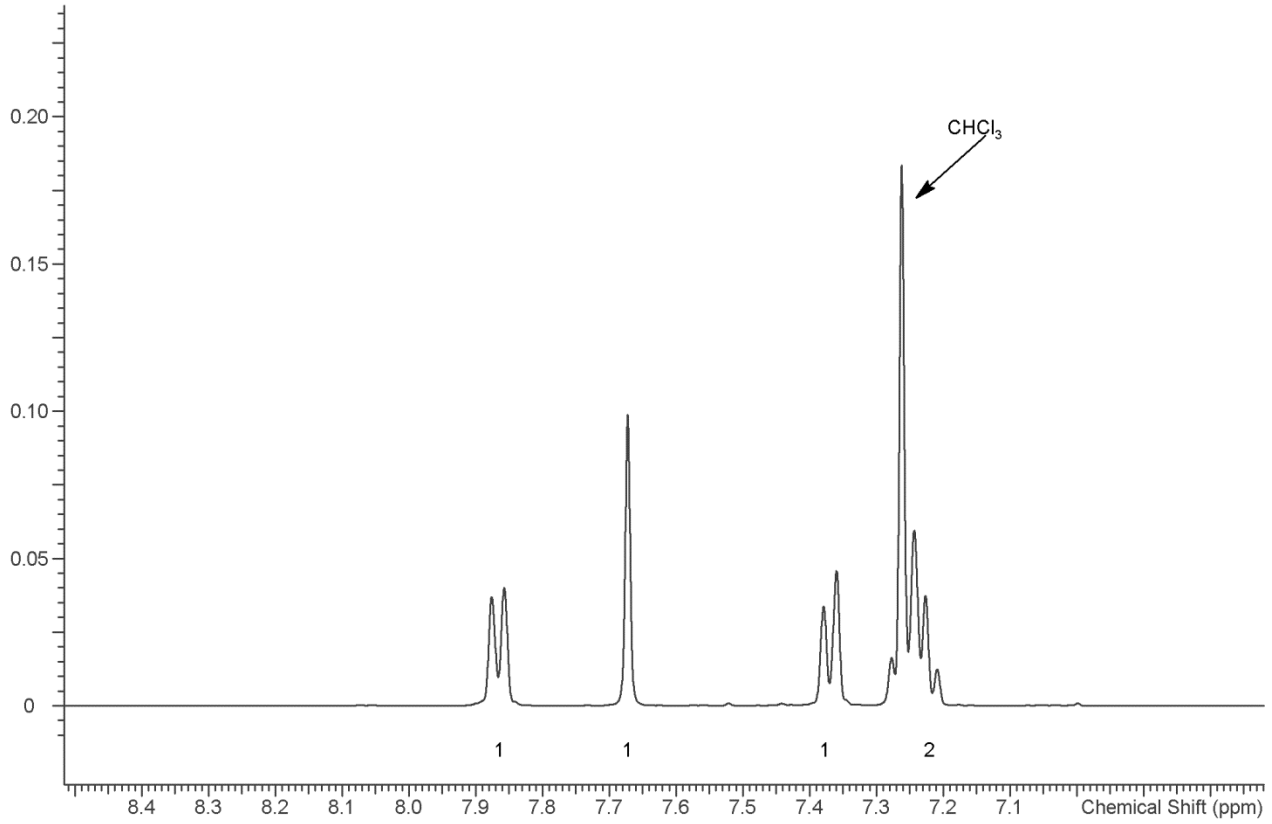
Sample Preparation: Dilute analyte to ~5 mg/mL in deuterochloroform ($CDCl_3$) containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

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

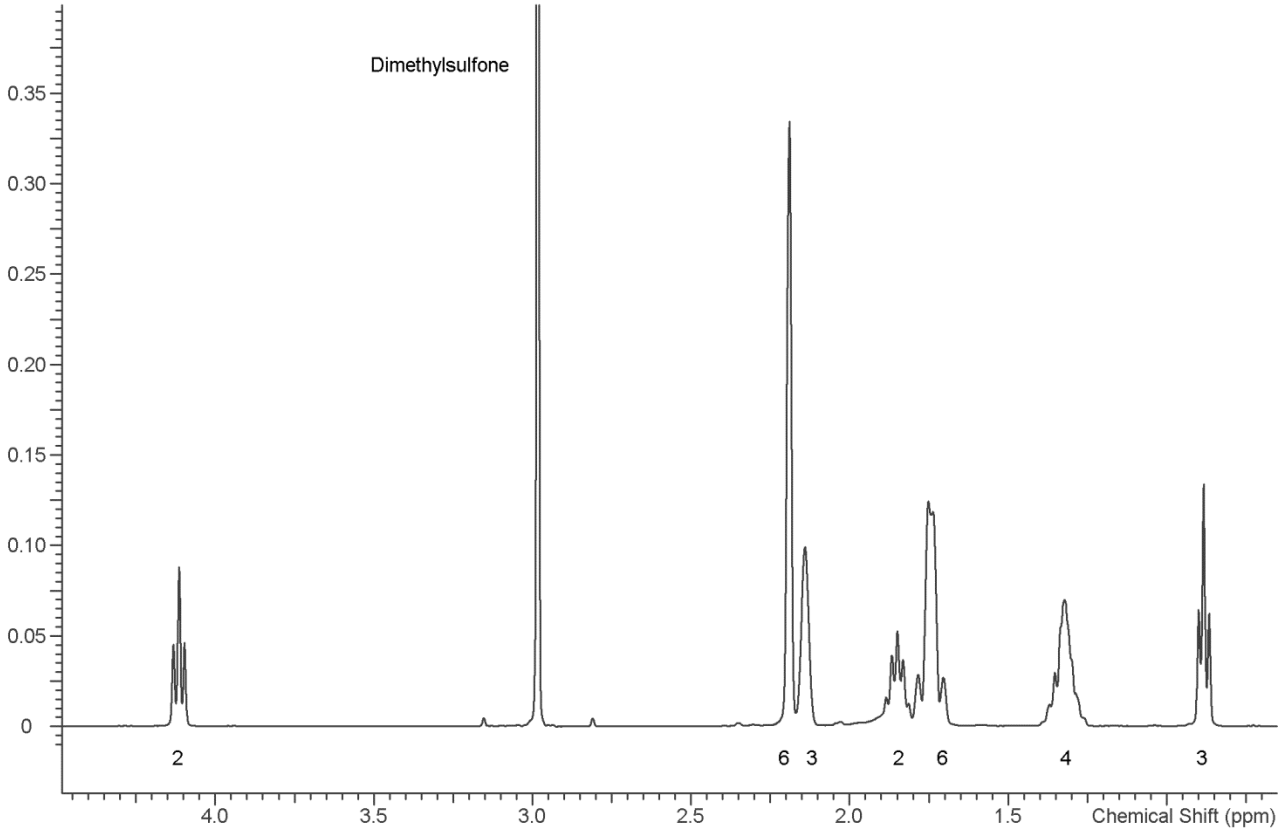
Parameters:
Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual



1H NMR: JWH-018 adamantyl carboxamide Lot # 0435618-27, $CDCl_3$; 400 MHz



1H NMR: JWH-018 adamantyl carboxamide Lot # 0435618-27, $CDCl_3$; 400 MHz

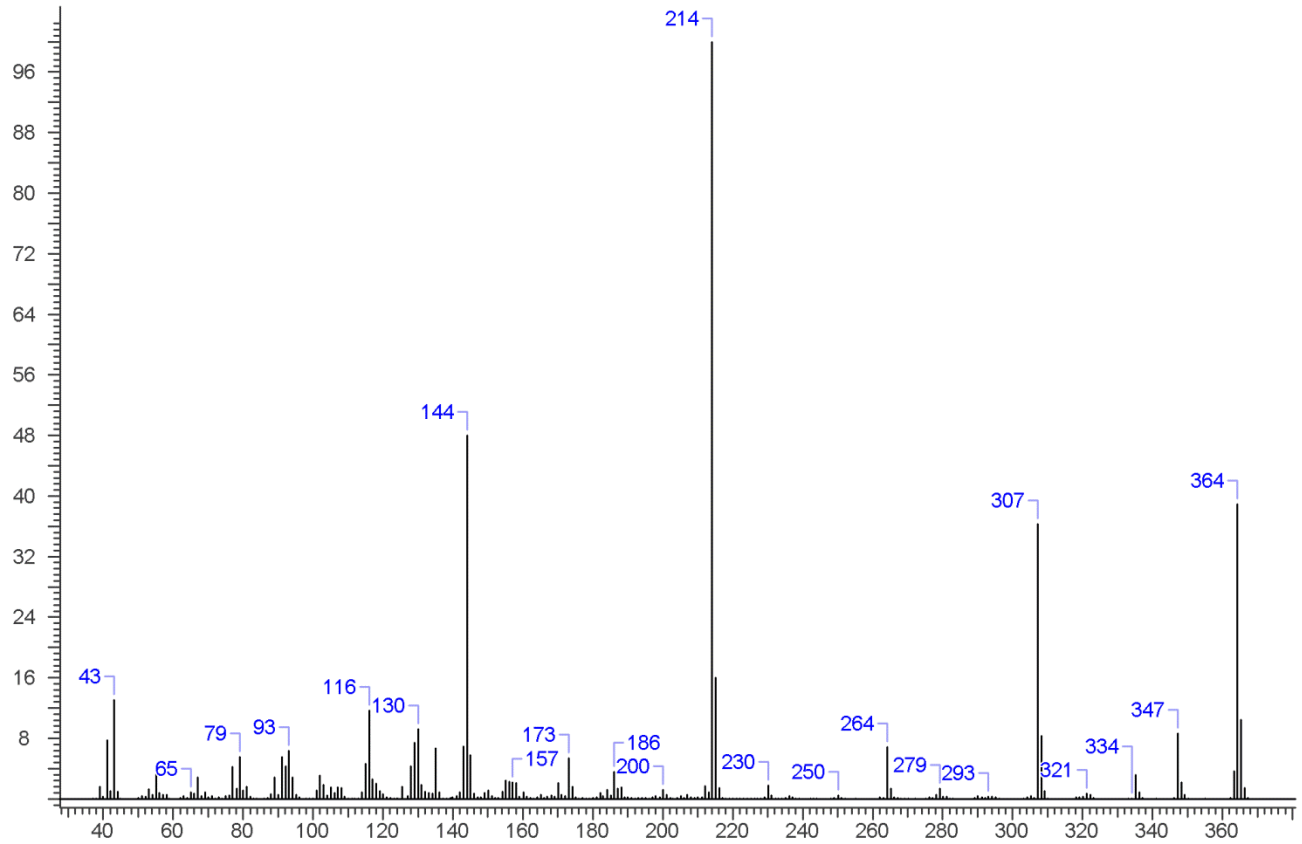


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~2 mg/mL in $CHCl_3$.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x .25mm x .25µm
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 25.0 min
Injection Parameters:	Split Ratio = 25:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	22.380 minutes

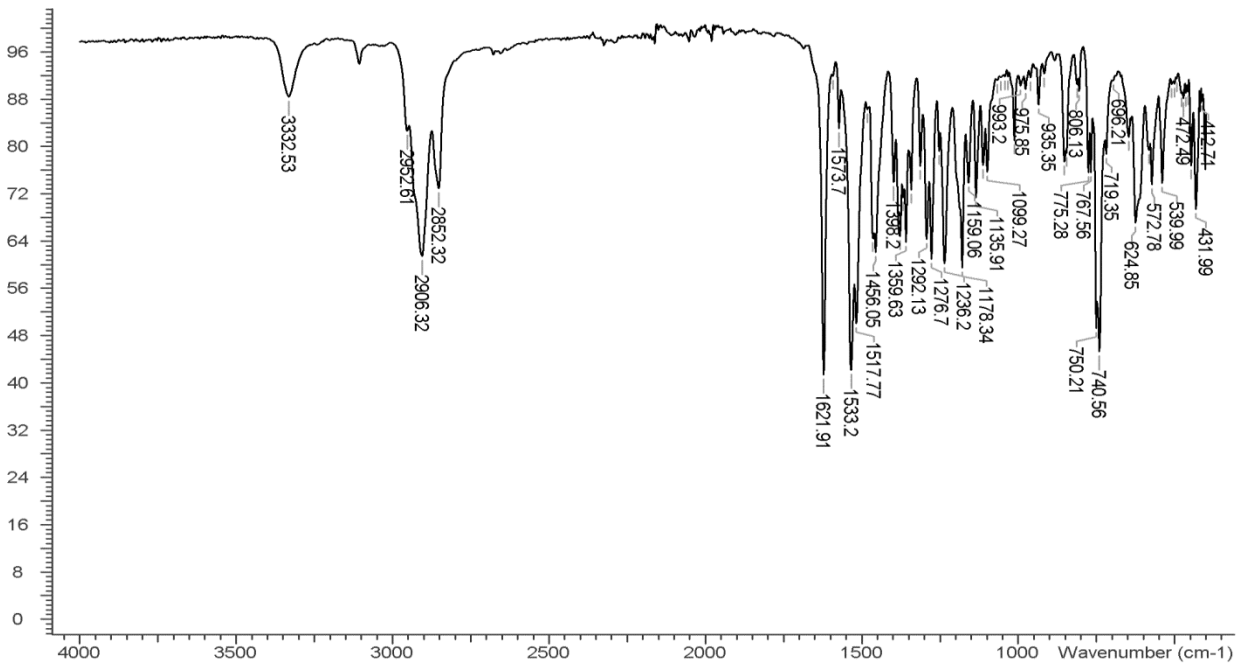
EI Mass Spectrum: JWH-018 adamantyl carboxamide Lot # 0435618-27



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): JWH-018 adamantyl carboxamide Lot # 0435618-27



FTIR ATR (Diamond, 3 Bounce): JWH-018 adamantyl carboxamide Lot # 0435618-27