

1. GENERAL INFORMATION

IUPAC Name:	2-(2-methoxyphenyl)-1-(1-pentyl-1 <i>H</i> -indol-3-yl)ethanone
CFR:	Schedule I
CAS #:	864445-43-2
Synonyms:	1-pentyl-3-(2-methoxyphenylacetyl)indole
Source:	DEA Reference Material Collection
Appearance:	Pink powder
Kovat's Index:	Pending
UV_{max} (nm):	218.1, 245.0, 296.7

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₂ H ₂₅ NO ₂	335	82.6

3. *ADDITIONAL RESOURCES*

Harris D, Hokanson S, Miller V. GC-MS Differentiation of Three Synthetic Cannabinoid Positional Isomers: JWH-250, JWH-302, and JWH-201. *Journal of the Clandestine Laboratory Investigating Chemists Association* 2011. 21(4): 23-32.

Nakajima J, Takahashi M, Seto T, Suzuki J. Identification and quantitation of cannabimimetic compound JWH-250 as an adulterant in products obtained via the Internet. *Forensic Toxicology* 2011. 29:51-55.

[Forendex](#)

[Wikipedia](#)

4. *QUALITATIVE DATA*

4.1 NUCLEAR MAGNETIC RESONANCE

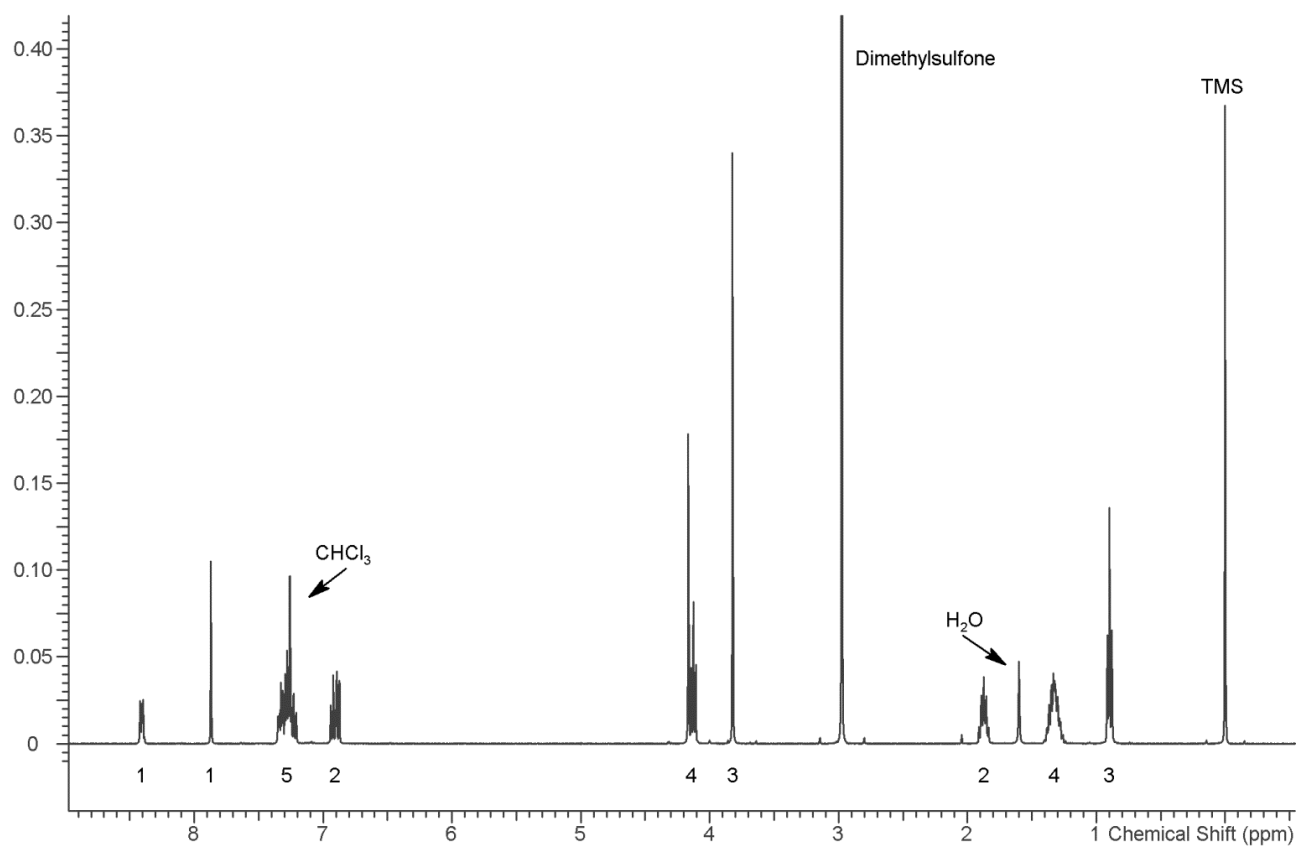
Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in deuteriochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

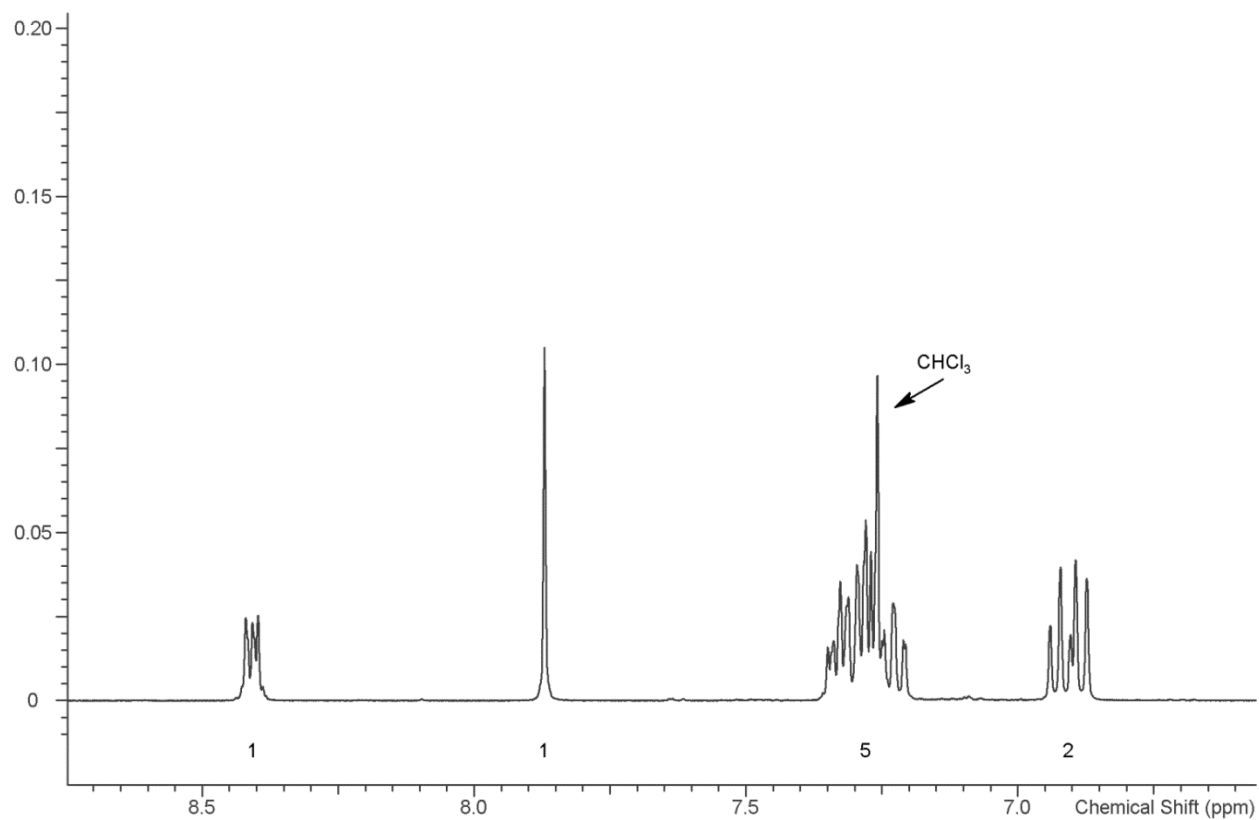
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

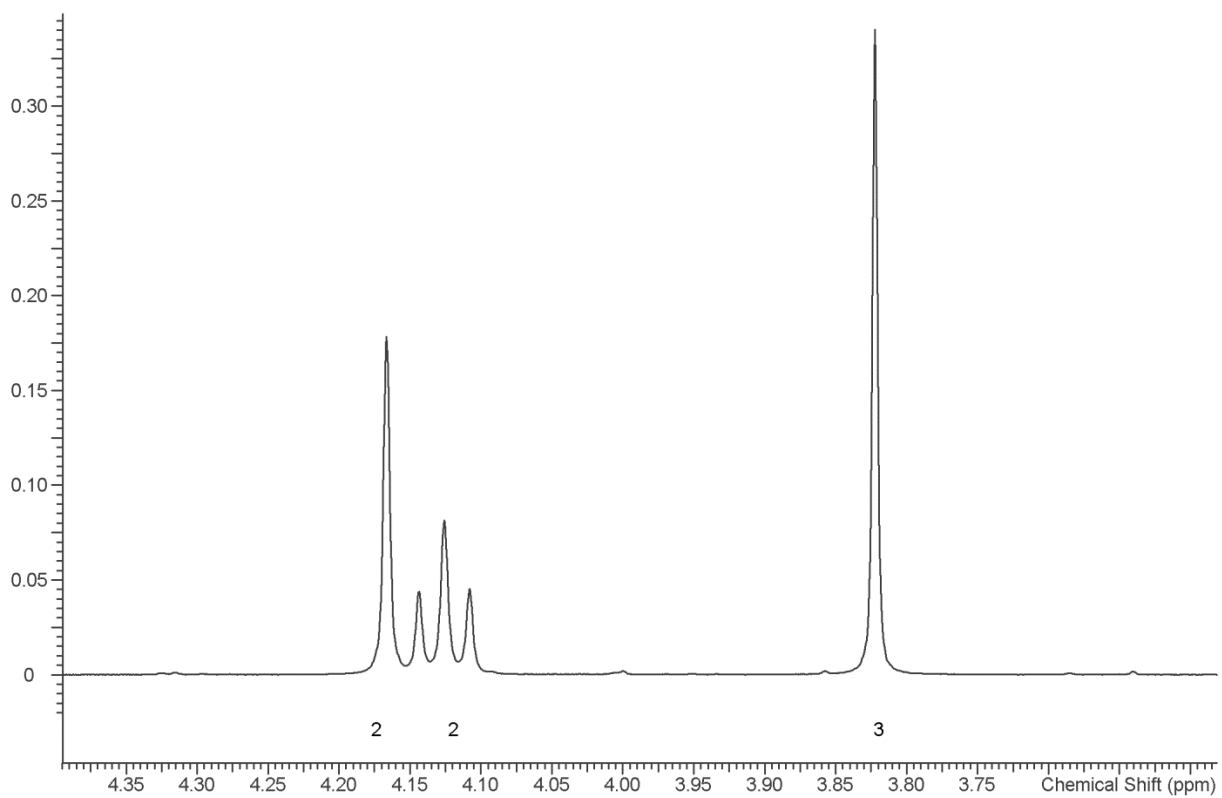
1H NMR: JWH-250 Lot # ALB055RC; CDCl₃; 400 MHz



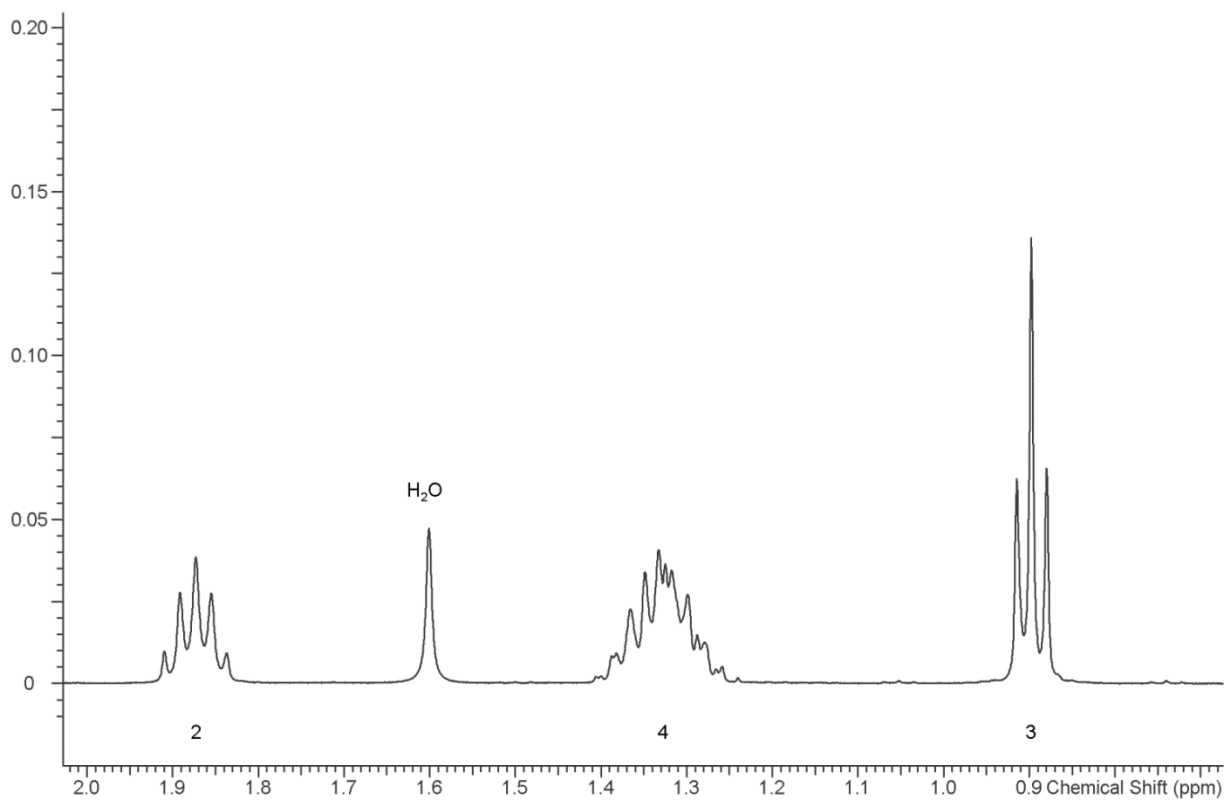
1H NMR: JWH-250 Lot # ALB055RC; CDCl₃; 400 MHz



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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 or equivalent; 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) 90°C initial temperature for 2.0 min

2) Ramp to 300°C at 14°C/min

3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

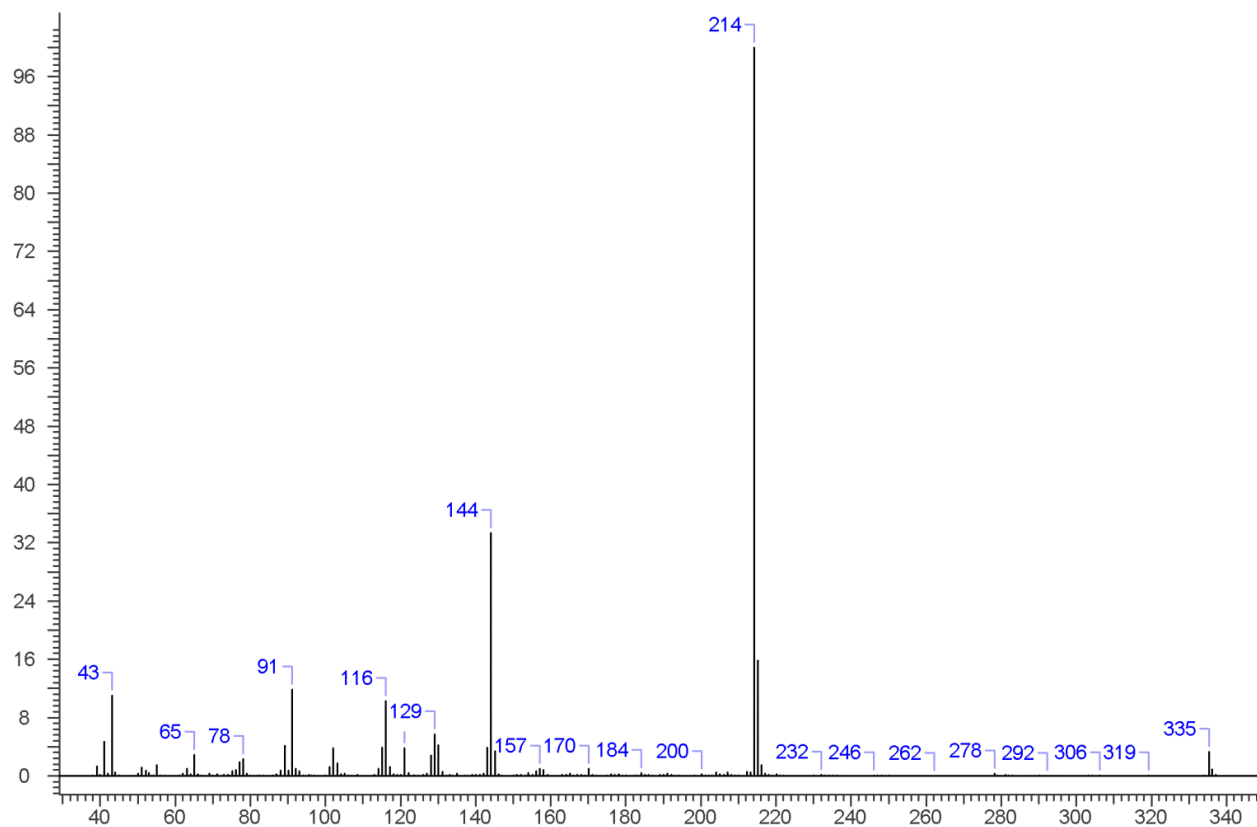
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 18.249 minutes

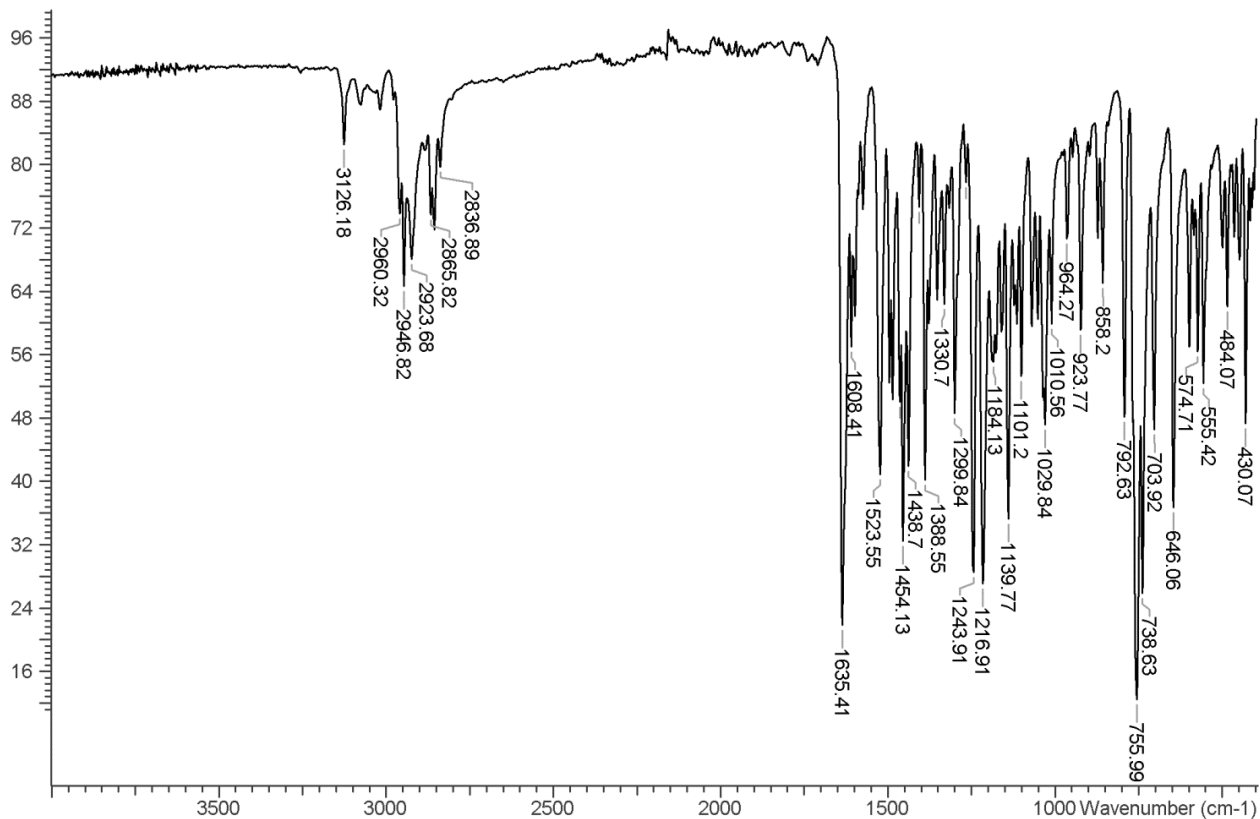
EI Mass Spectrum: JWH-250 Lot # ALB055RC



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-250 Lot # ALB055RC



FTIR ATR (Diamond, 3 Bounce): JWH-250 Lot # ALB055RC

