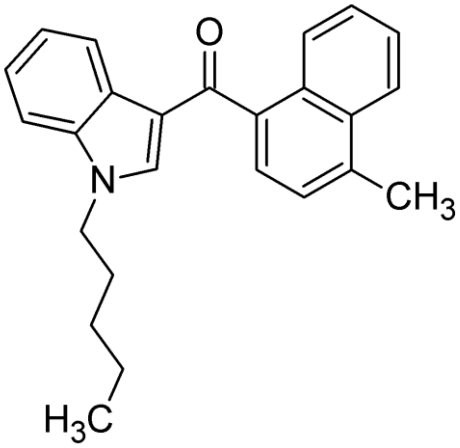
JWH-122

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name: (4-methylnaphthalen-1-yl)(1-pentyl-1*H*-indol-3-yl)methanone

CAS #: 619294-47-2

Synonyms: (4-methyl-1-naphthyl)-(1-pentylindol-3-yl)methanone,
(4-methyl-1-naphthalenyl)-(1-pentyl-3-indolyl)methanone,
(4-methylnaphthalen-1-yl)-(1-pentylindol-3-yl)methanone,
(1-amylindol-3-yl)-(4-methyl-1-naphthyl)methanone

Source: DEA Reference Material Collection

Appearance: Tan powder

UV_{max}: 221.8, 314.6

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{25}H_{25}NO$	355	88.9

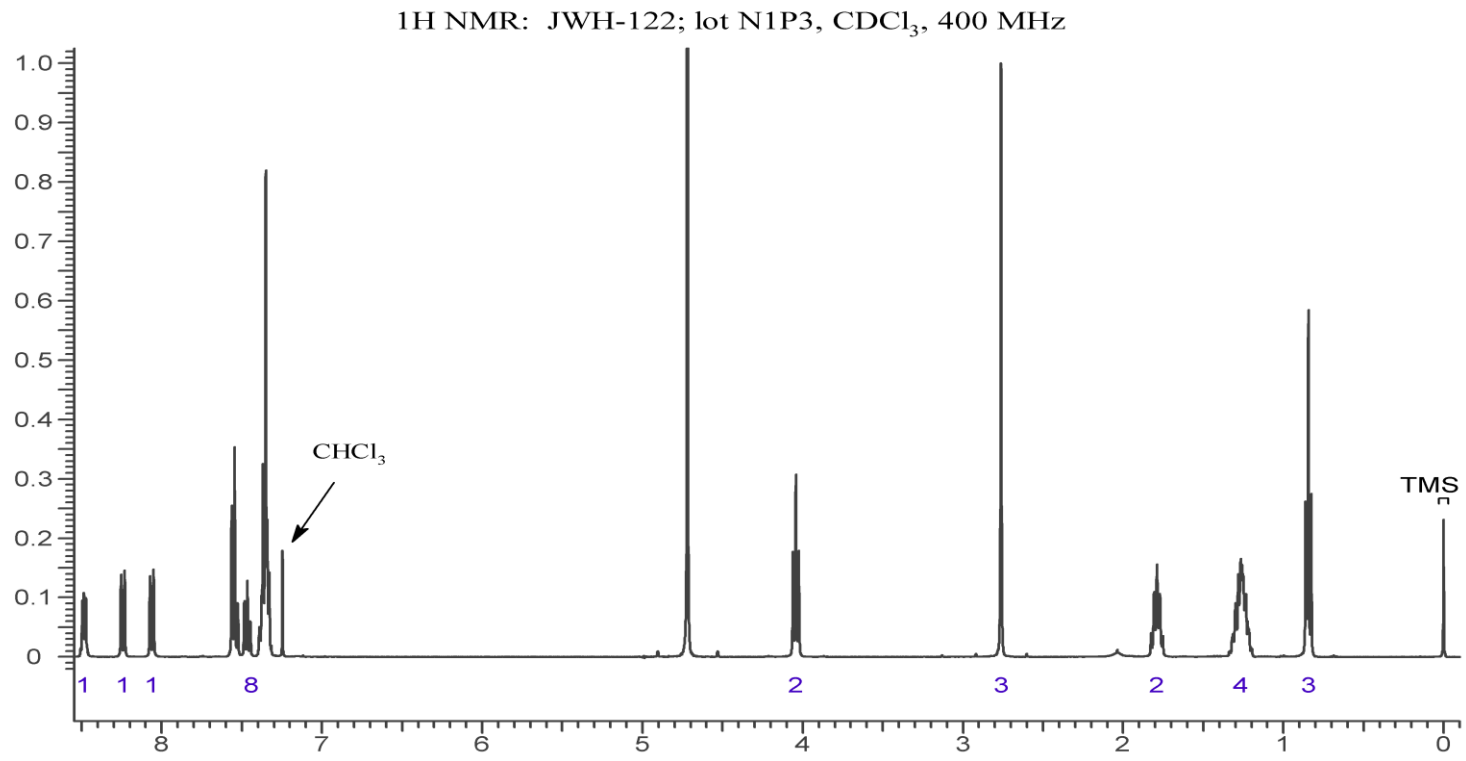
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

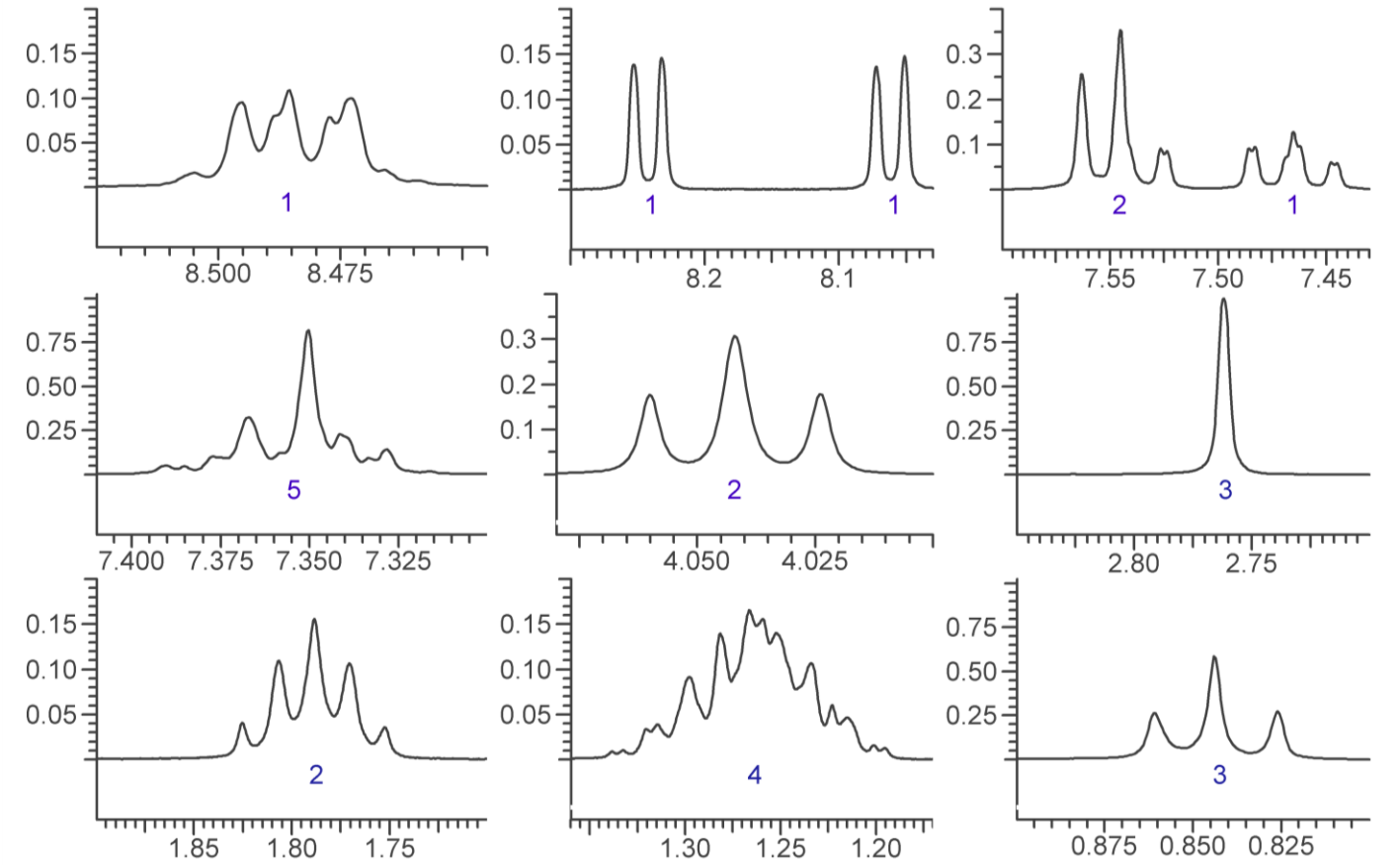
Method NMR $CDCl_3$

Sample Preparation: Dilute analyte to ~10 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and methenamine 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-122; lot N1P3, $CDCl_3$, 400 MHz

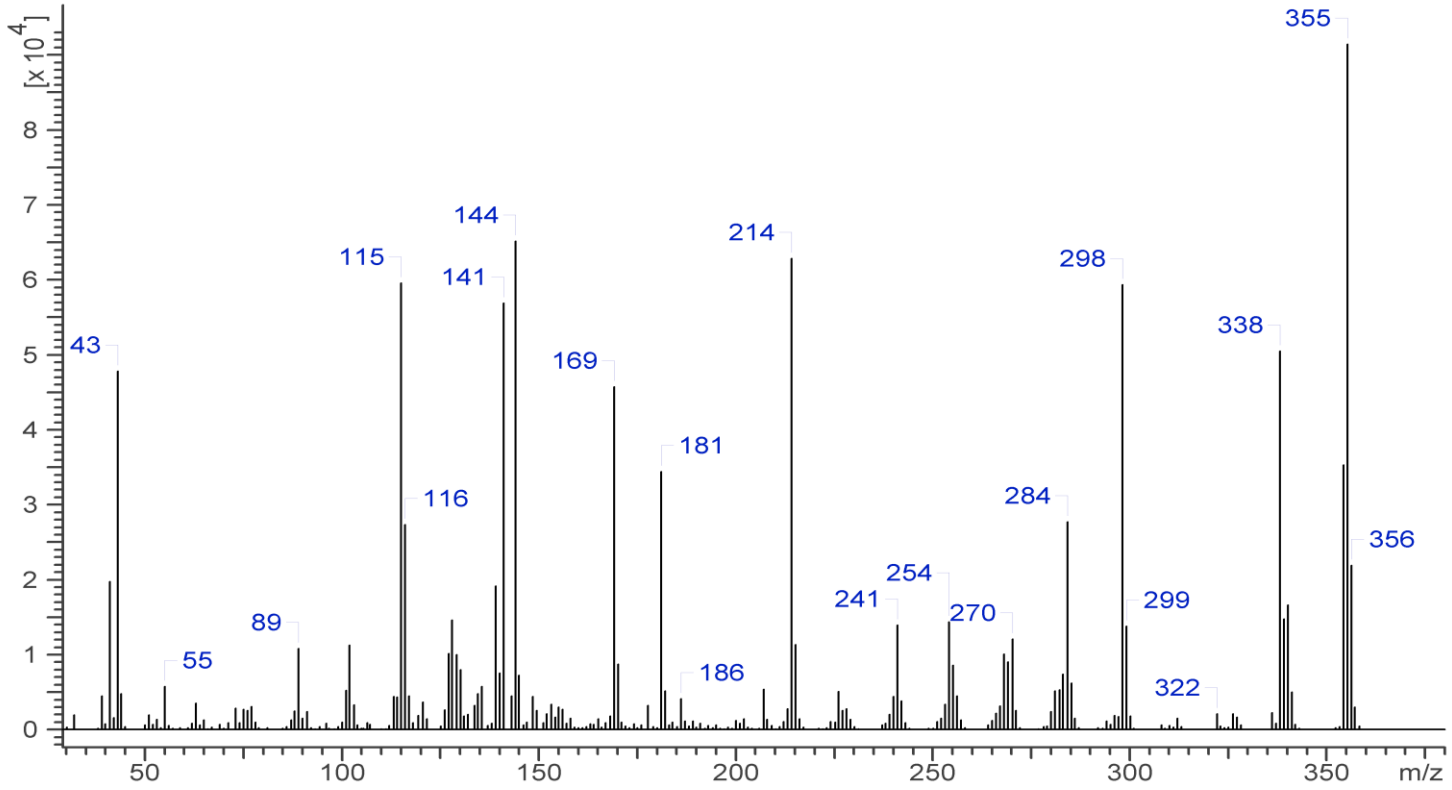


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL into methanol.

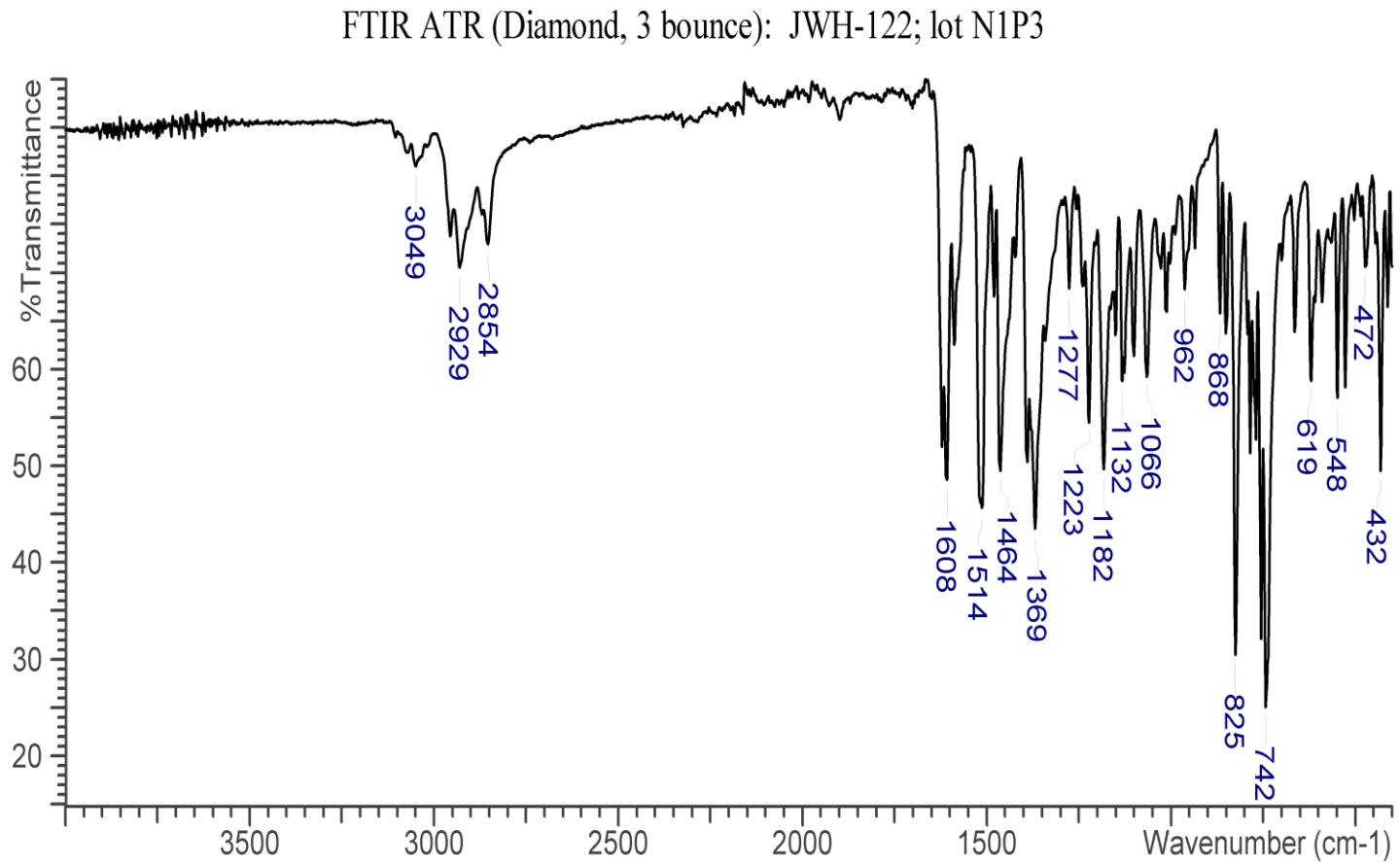
Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12°C/min 3) Hold final temperature for 9.0 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:	21.420 minutes

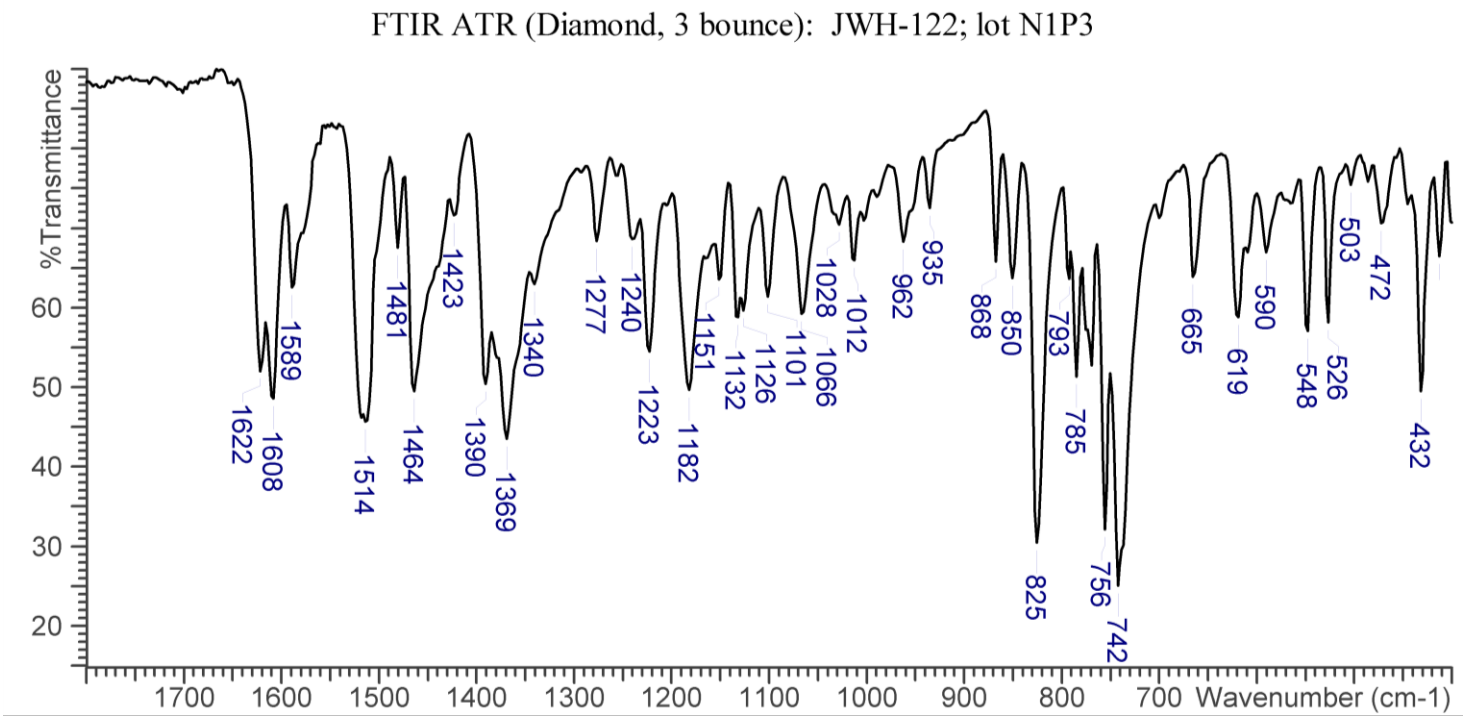
EI Mass Spectrum: JWH-122; lot N1P3



3.3 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





4. ADDITIONAL RESOURCES

Nakajima J, Takahashi M, Seto T, *et al*. Identification and quantitation of two benzoylindoles AM-694 and (4-methoxyphenyl)(1-pentyl-1H-indol-3-yl)methanone, and three cannabimimetic naphthoylindoles JWH-210, JWH-122, and JWH-019 as adulterants in illegal products obtained via the internet. J Forensic Toxicol. 2011; 29(2): 95-110.

Ernst L, Schiebel HM, Theuring C, Lindigkeit R, Beuerle T. Identification and characterization of JWH-122 used as new ingredient in "Spice-like" herbal incenses. *J Forensic Science International.* 2011; 208: E31-E35.

De Freitas GBL, da Silva LL, Romeiro NC, Fraga CAM. Development of CoMFA and CoMSIA models of affinity and selectivity for indole ligands of cannabinoid CB1 and CB2 receptors. *Eur. J. Med. Chem*. 2009; 44(6): 2482-2496.

Tuccinardi T, Ferrarini PL, Manera C, Ortore G, Saccomanni G, Martinelli A. Cannabinoid CB2/CB1 Selectivity. Receptor Modeling and Automated Docking Analysis. *J. Med. Chem.* 2006; 49(3): 984-994.

Martin BR, Huffman JW, inventors; CB2-selective cannabinoid analogues. US patent 2005-0009903 A1. January 13, 2005.

Huffman JW, Zengin G, Wu, MJ, *et al*. Structure-activity relationships for 1-alkyl-3-(1-naphthoyl)indoles at the cannabinoid CB1 and CB2 receptors: steric and electronic effects of naphthoyl substituents. New highly selective CB2 receptor agonists. *Bioorg. Med. Chem.* 2004; 13(1): 89-112.

Huffman JW, Mabon R, Wu, MJ, *et al*. 3-Indolyl-1-naphthylmethanes: new cannabimimetic indoles provide evidence for aromatic stacking interactions with the CB1 cannabinoid receptor. *Bioorg. Med. Chem*. 2003; 11(4): 539-549.

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