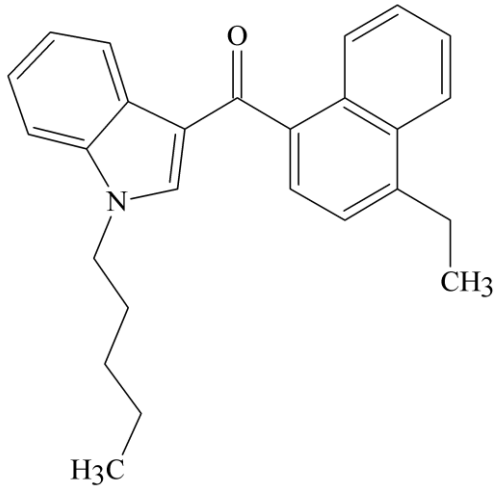
JWH-210

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



1. GENERAL INFORMATION

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

CAS #: 824959-81-1

Synonyms: n/a

Source: DEA Reference Material Collection

Appearance: Pink powder

UV_{max}: Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{26}H_{27}NO$	369	90.2

3. QUALITATIVE DATA

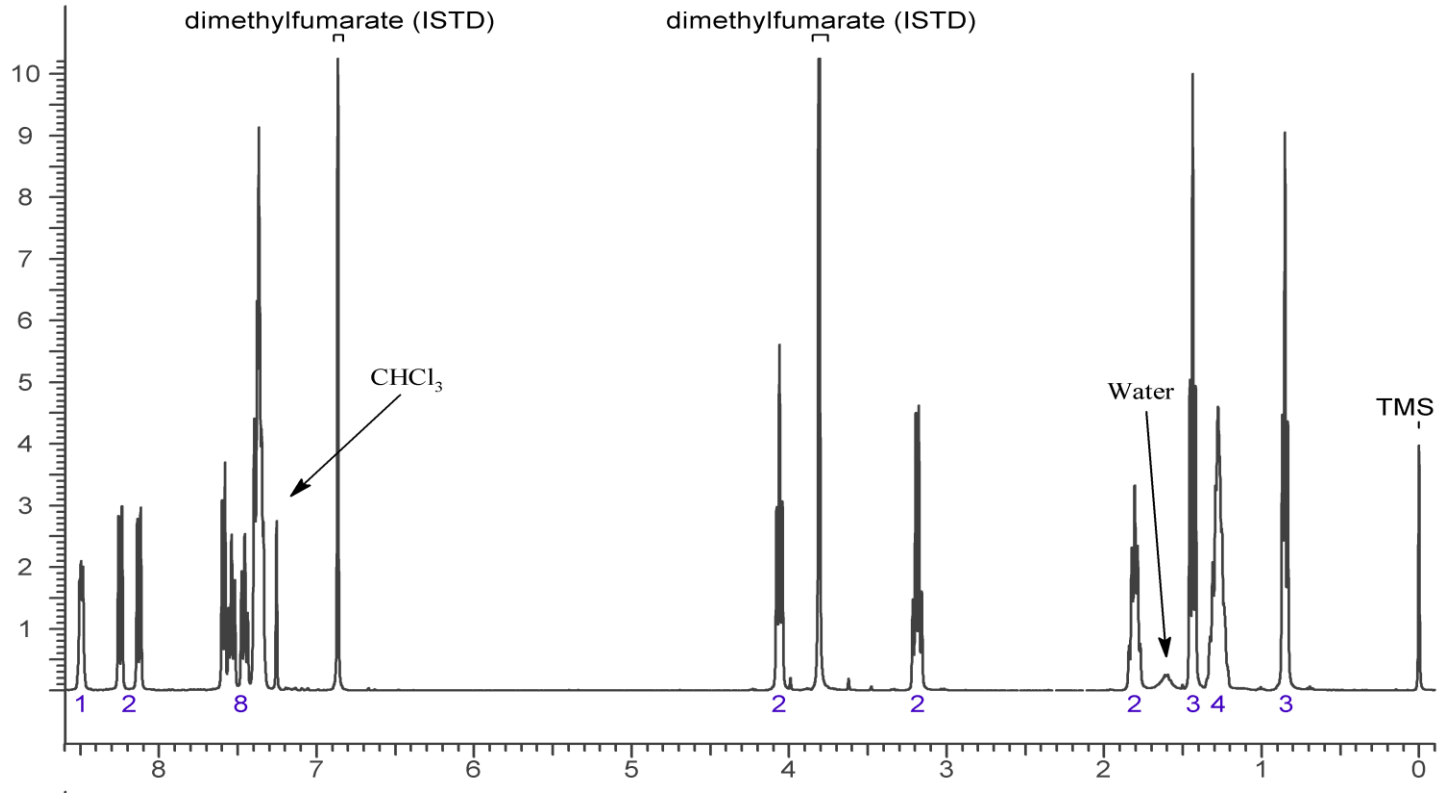
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

Sample Preparation: Dilute analyte to ~10 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and 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

^{1}H NMR: JWH-210; lot N1P36EMG; $CDCl_3$; 400 MHz



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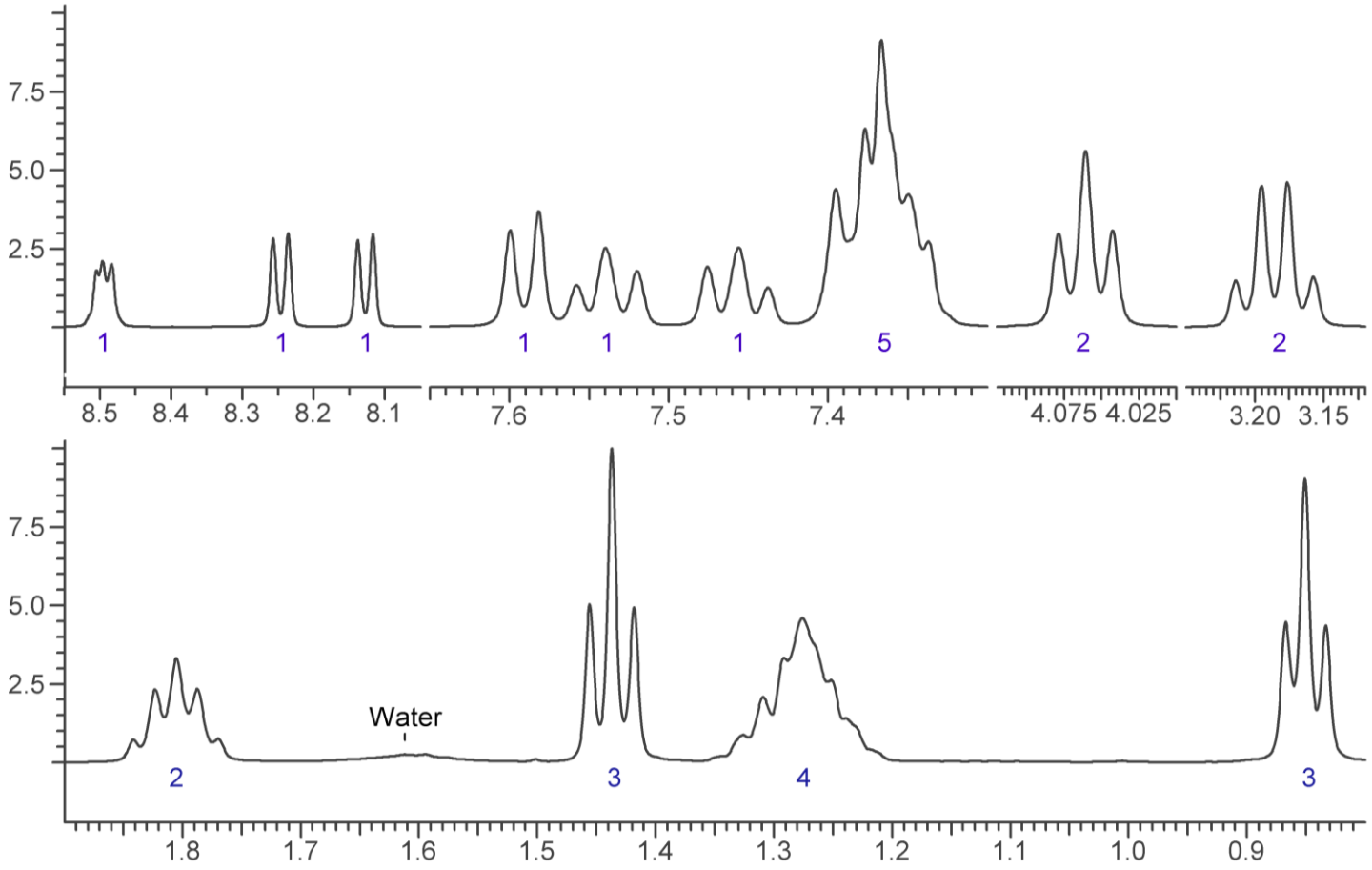
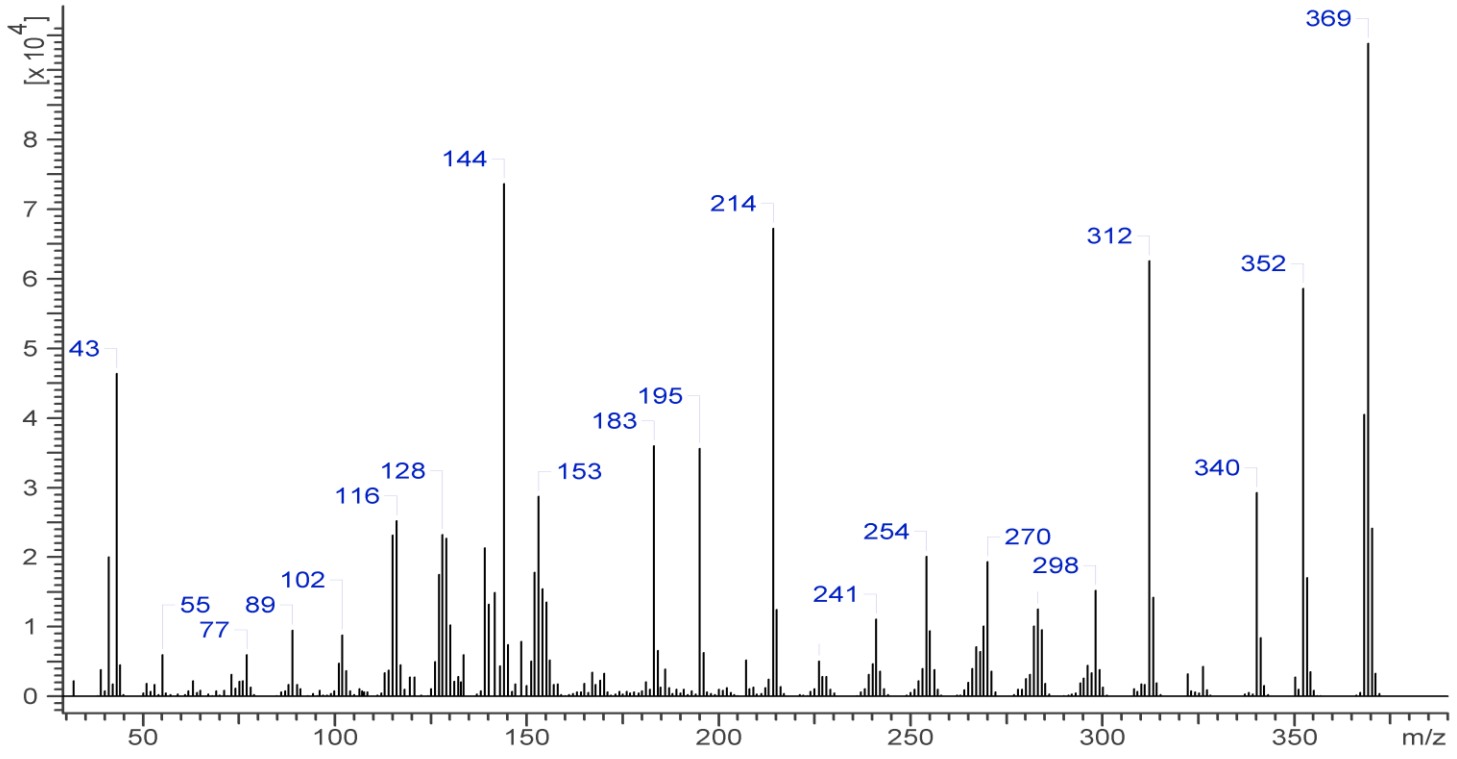


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

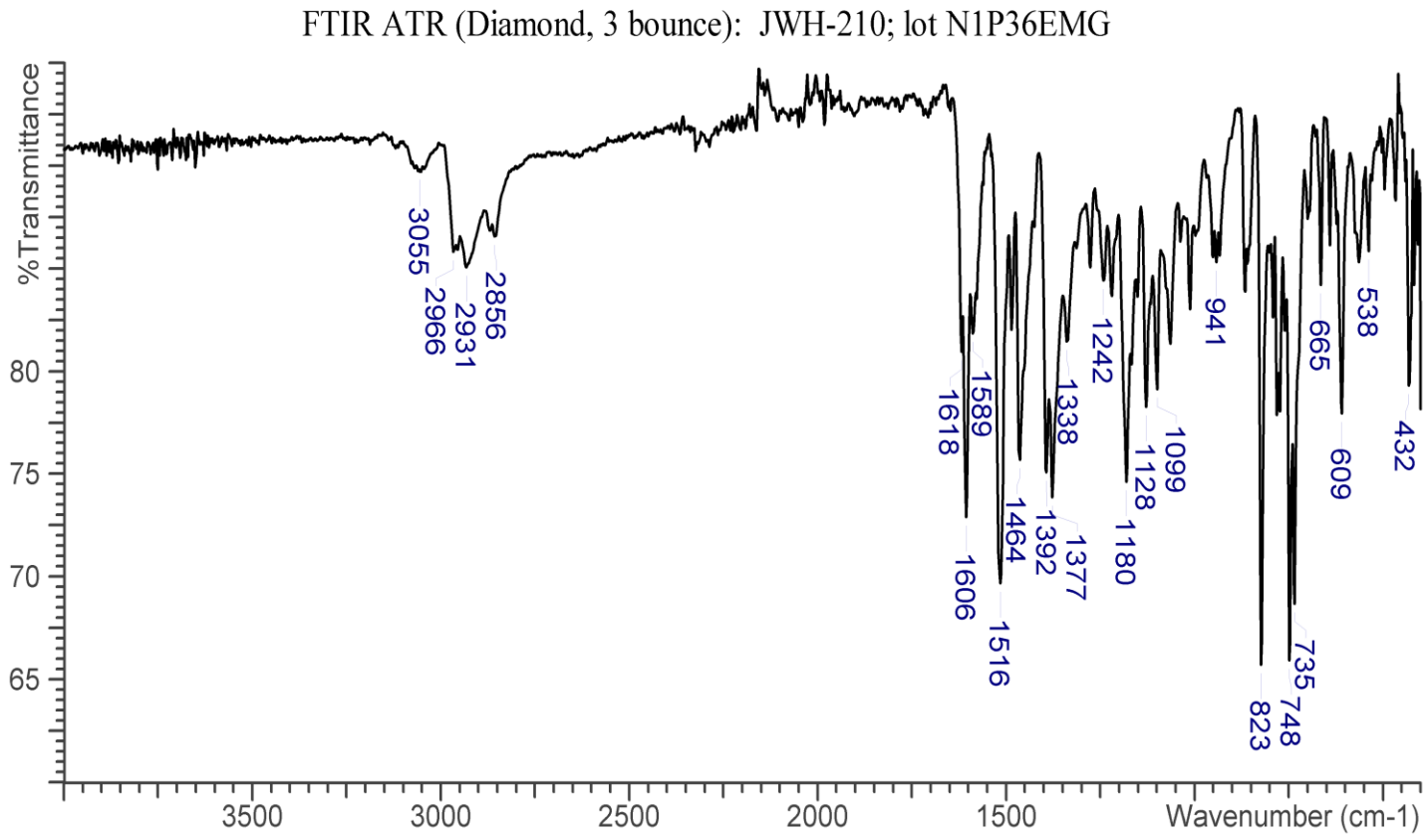
Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp 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:	22.150 minutes

EI Mass Spectrum: JWH-210; lot N1P36EMG

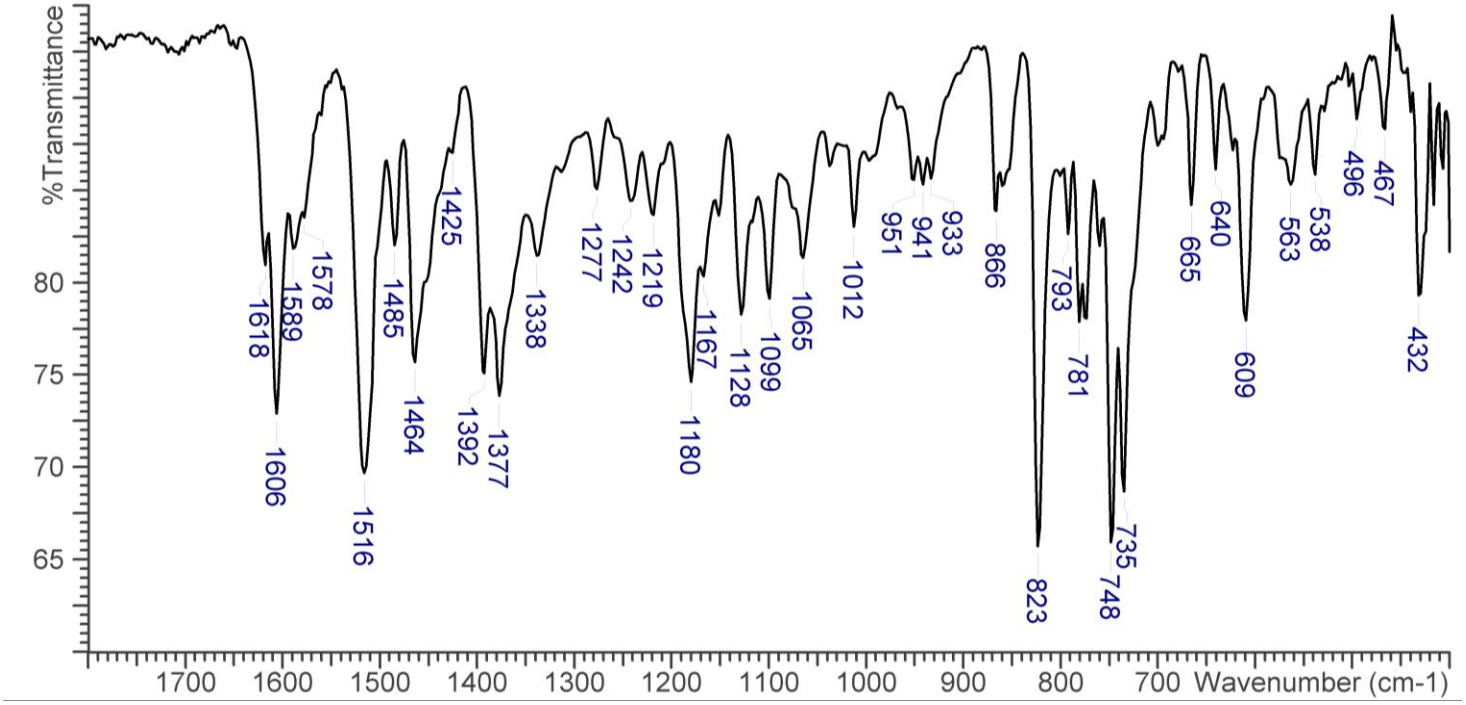


3.3 INFRARED SPECTROSCOPY (FTIR)

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



FTIR ATR (Diamond, 3 bounce): JWH-210; lot N1P36EMG



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.

Rituparna S, Mahmood SK, Ravikumar M. Quantitative structure activity relationship of indole-carbaldehyde derivatives as cannabinoid receptor 2 agonists. *Lett. Drug Des. Discovery*. 2009**;** 6(8): 599-619.

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.

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

Martin BR, Huffman JW, inventors; Preparation of cannabinoids and their indole analogs with CB2 cannabinoid receptor selectivity for use in pharmaceutical compositions for the treatment of pain and cancer. US patent 20050009903 A1. January 13, 2005.

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