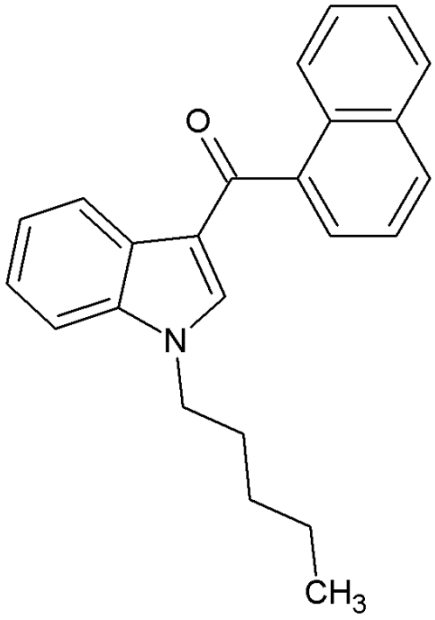


1. GENERAL INFORMATION

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

CFR: Schedule I

CAS #: 209414-07-3

Synonyms: AM678, 1-pentyl-3-(1-naphthoyl)indole

Source: DEA Reference Material Collection

Appearance: Off-white powder

Kovat's Index: Pending

UV_{max}: 218.1, 314.6 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{24}H_{23}NO$	341	51.9

3. ADDITIONAL RESOURCES

Kneisel S, Westphal F, Rosner P, et.al. Cannabinoidmimetika: Massenspektren und IR-ATR-Spektren neuer Verbindungen aus den Jahren 2009/2010. *Toxichem Krimtech.* 2011; 78(1):23-35.

Forendex

Wikipedia

4. QUALITATIVE DATA

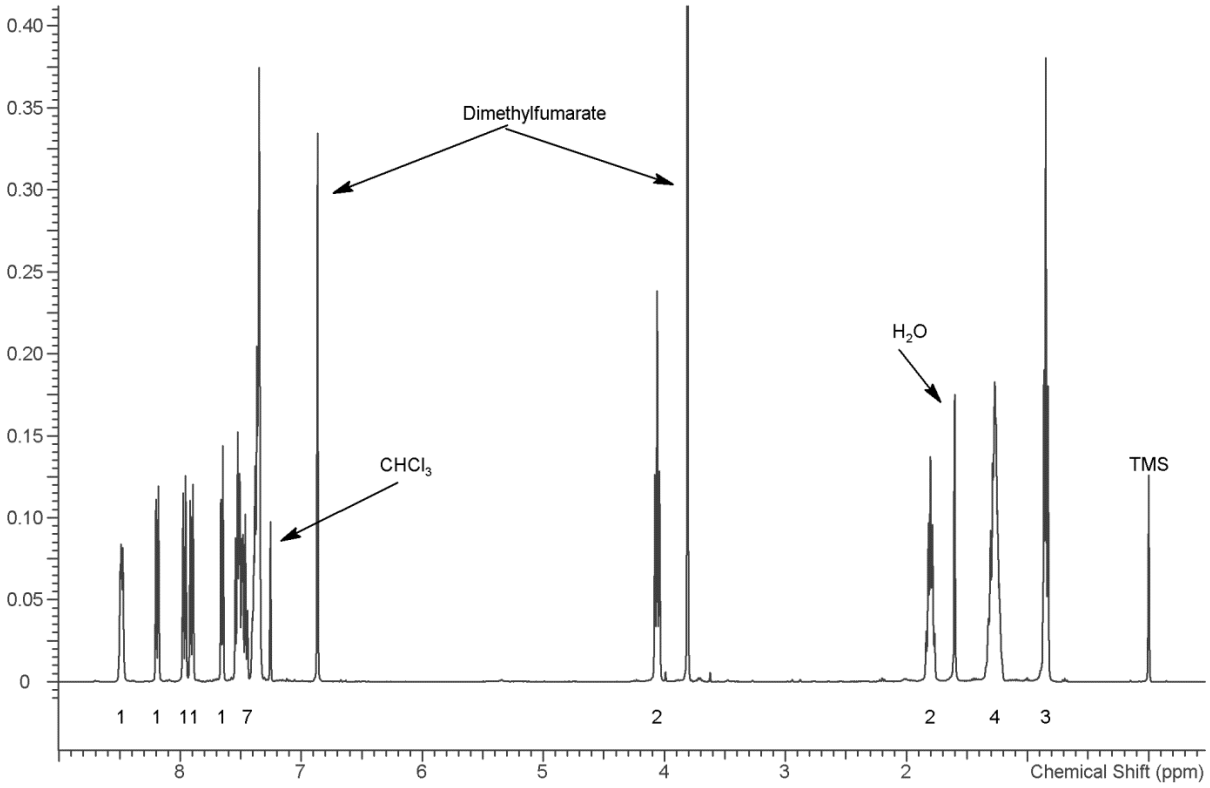
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

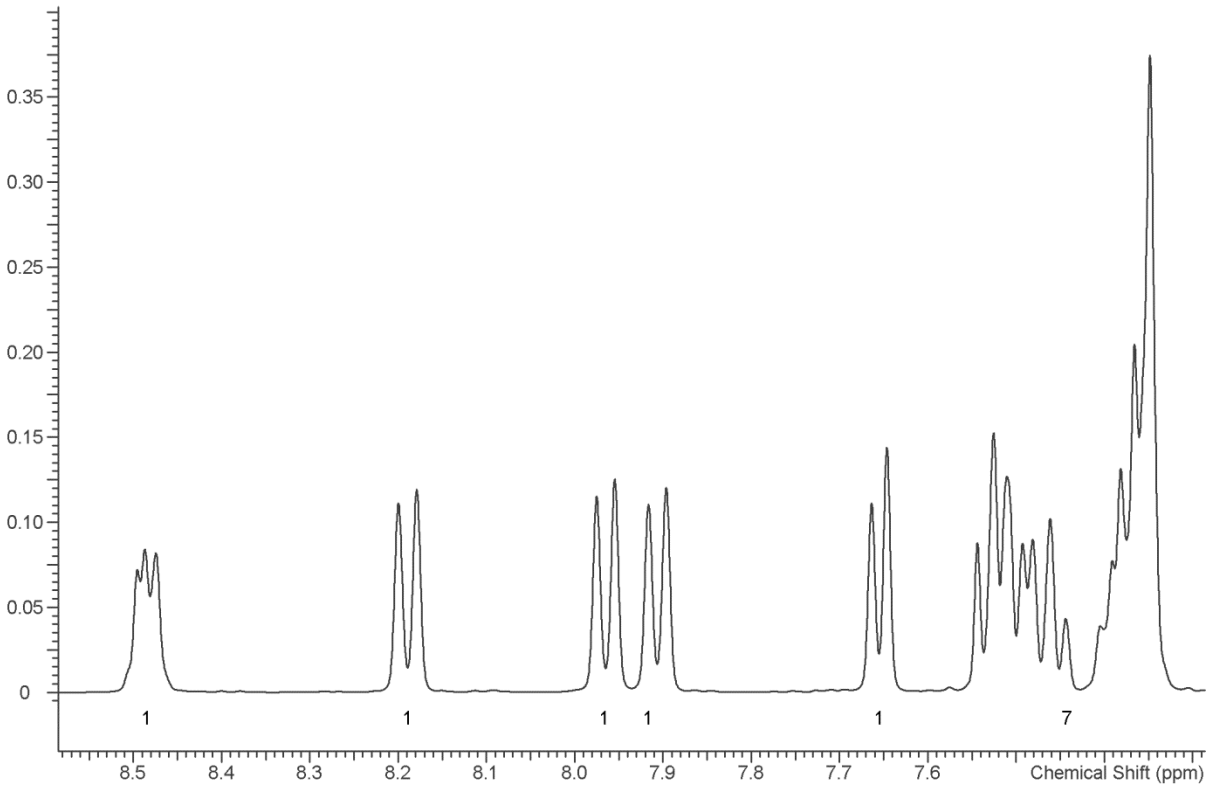
Sample Preparation: Dilute analyte to ~20 mg/mL in deuterochloroform ($CDCl_3$) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

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

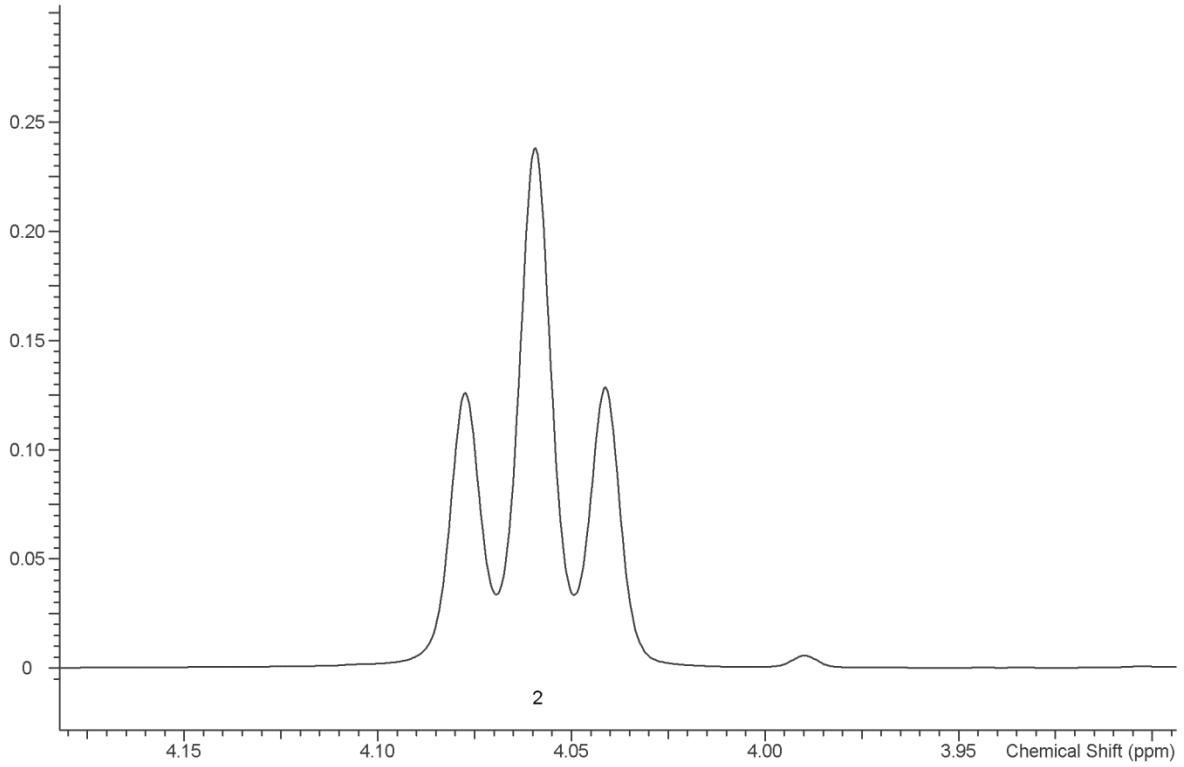
1H NMR: JWH-018 Lot # ALB045RC/183-1; $CDCl_3$; 400MHz



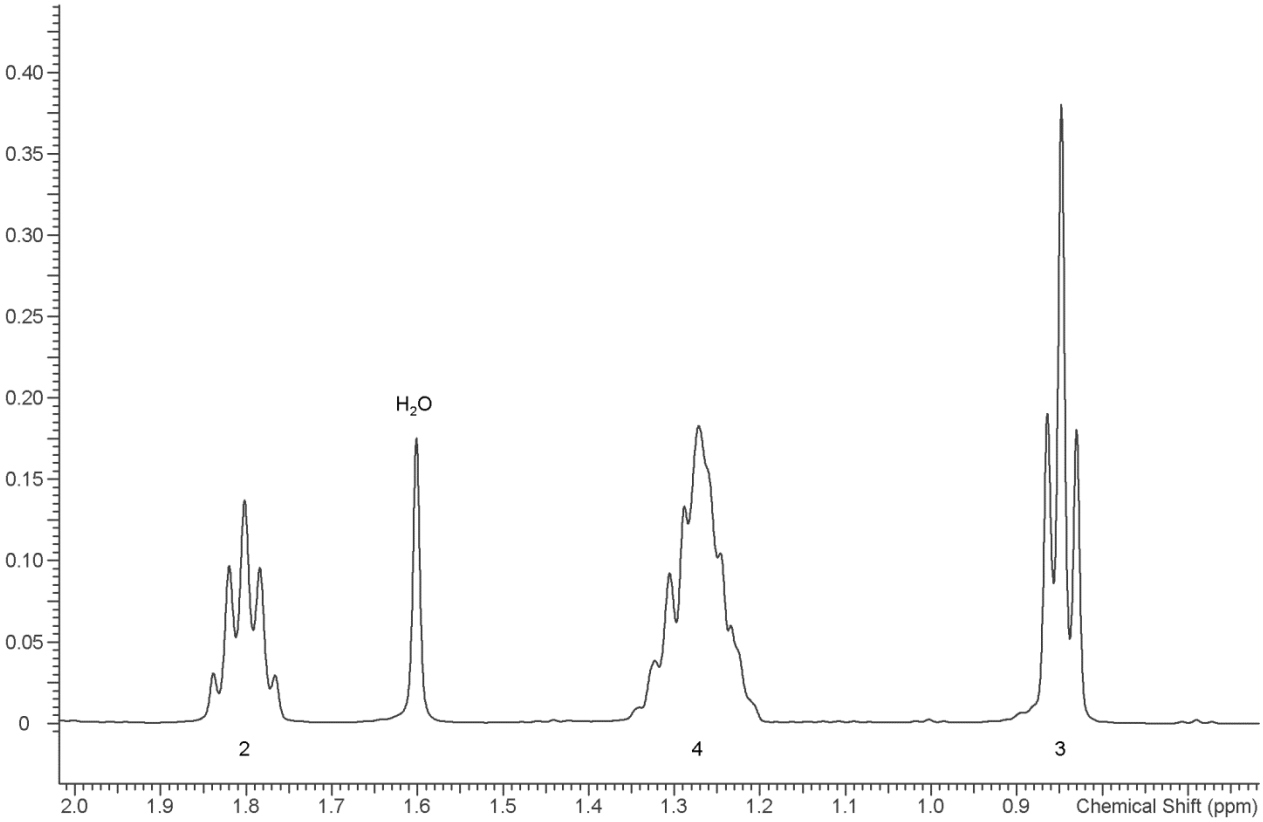
1H NMR: JWH-018 Lot # ALB045RC/183-1; $CDCl_3$; 400MHz



1H NMR: JWH-018 Lot # ALB045RC/183-1; $CDCl_3$; 400MHz



1H NMR: JWH-018 Lot # ALB045RC/183-1; $CDCl_3$; 400MHz

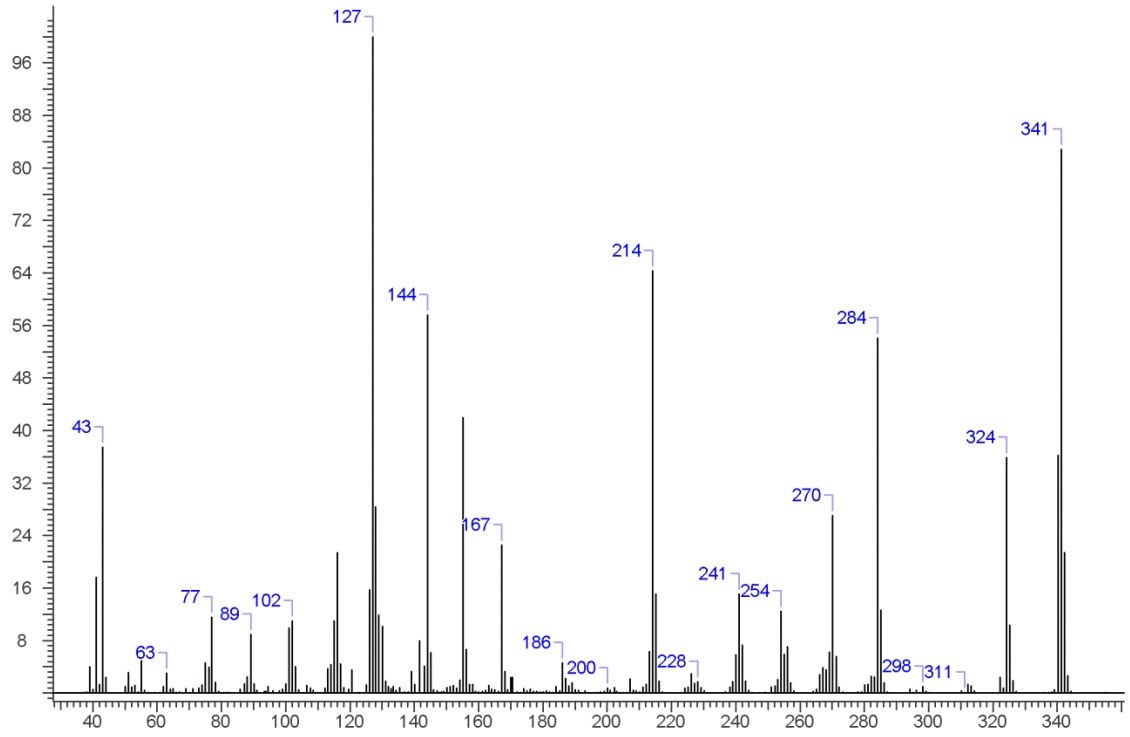


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 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) 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 µL injected
MS Parameters:	Mass scan range: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	20.011 minutes

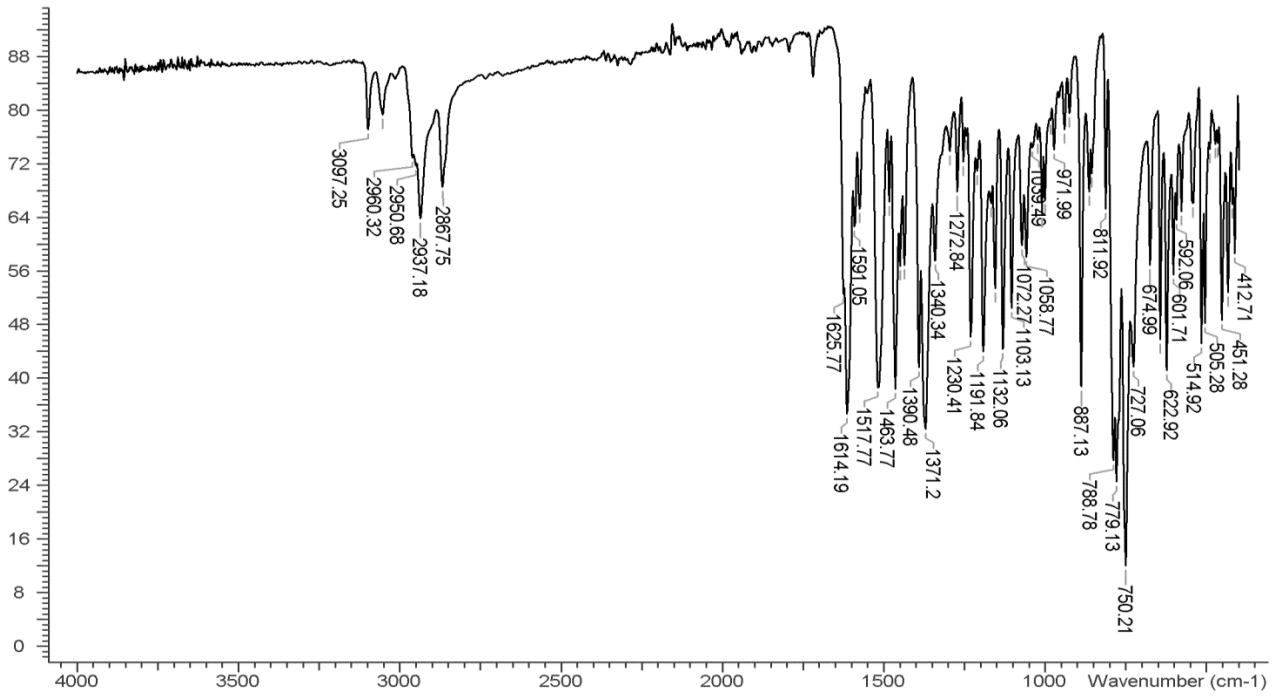
EI Mass Spectrum: JWH-018 Lot # ALB045RC/183-1



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 Lot # ALB045RC/183-1



FTIR ATR (Diamond, 3 Bounce): JWH-018 Lot # ALB045RC/183-1