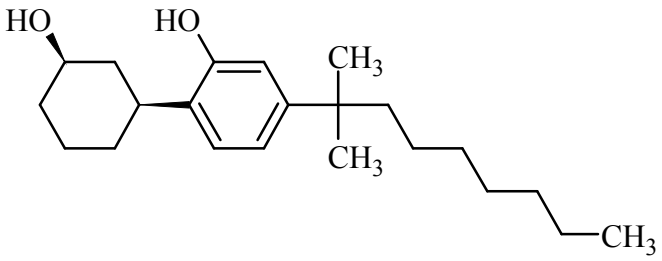
CP 47,497-C8-homolog

Latest Revision: August 23, 2013



1. GENERAL INFORMATION

IUPAC Name: *rel*-2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methylnonan-2-yl)phenol

CFR: Schedule I

CAS#: 70434-92-3

Synonyms: (±)-CP 47,497-C8-homolog, (C8)-CP 47,497, Cannabicyclohexanol, 5-(1,1-dimethyloctyl)-2-[(1R,3S)-3-hydroxycyclohexyl]-phenol

Source: DEA Reference Material Collection

Appearance: White powder

Kovat's Index: Pending

UV_{max} (nm): 274.5

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
CP 47,497-C8-homolog	$C_{22}H_{36}O_2$	332	89.4

3. ADDITIONAL RESOURCES

Forendex

Wikipedia

Uchiyama, N.; Kikura-Hanajiri, R.; Ogata, J.; Goda, Y. Chemical analysis of synthetic cannabinoids as designer drugs in herbal products. For. Sci. Int. **2010**, *198*, 31-38.

4. QUALITATIVE DATA

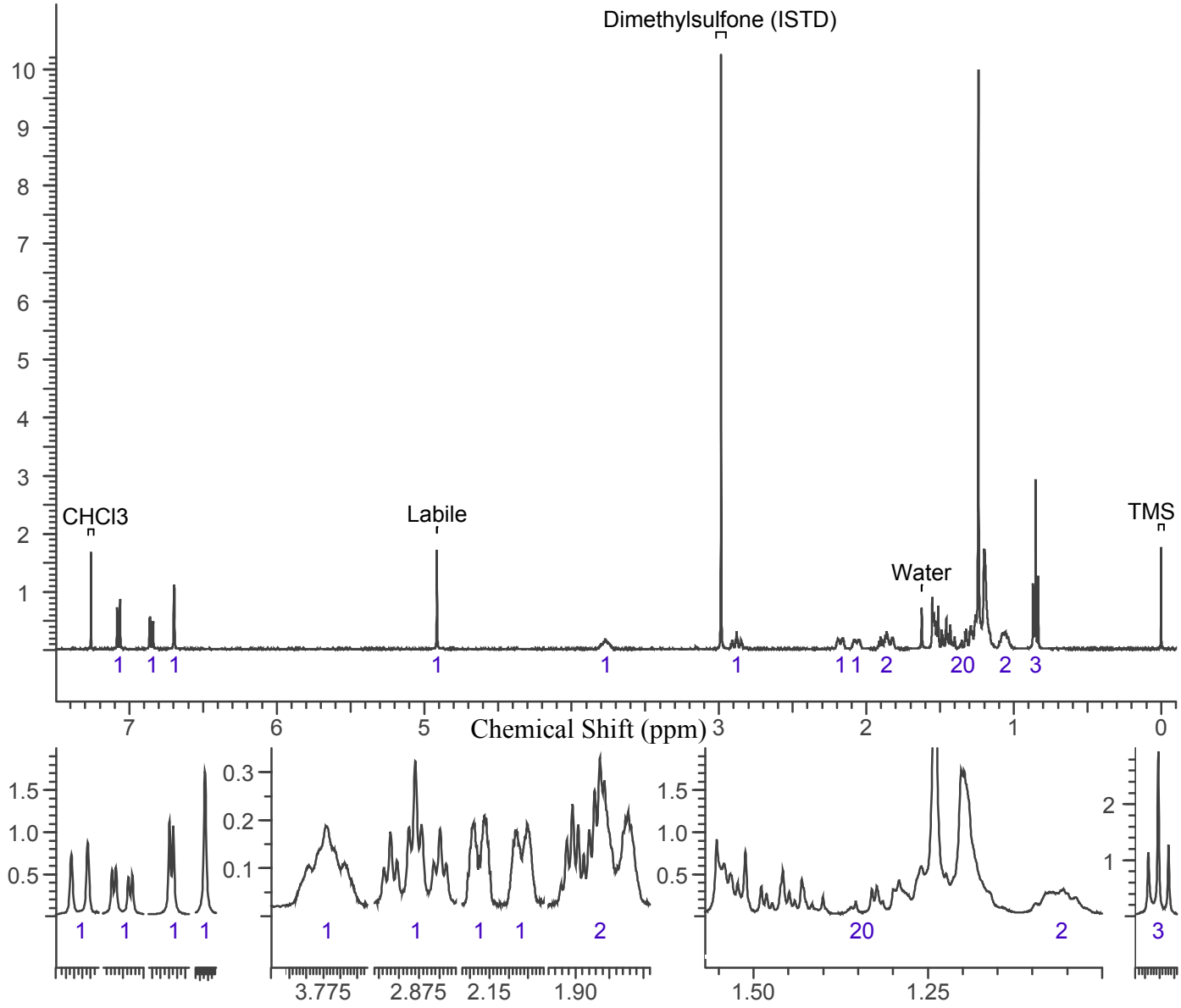
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

Sample Preparation: Dilute analyte to ~5 mg/mL in $CDCl_3$ 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: CP 47,497-C8-homolog; Lot 0425163-4; $CDCl_3$; 400 MHz

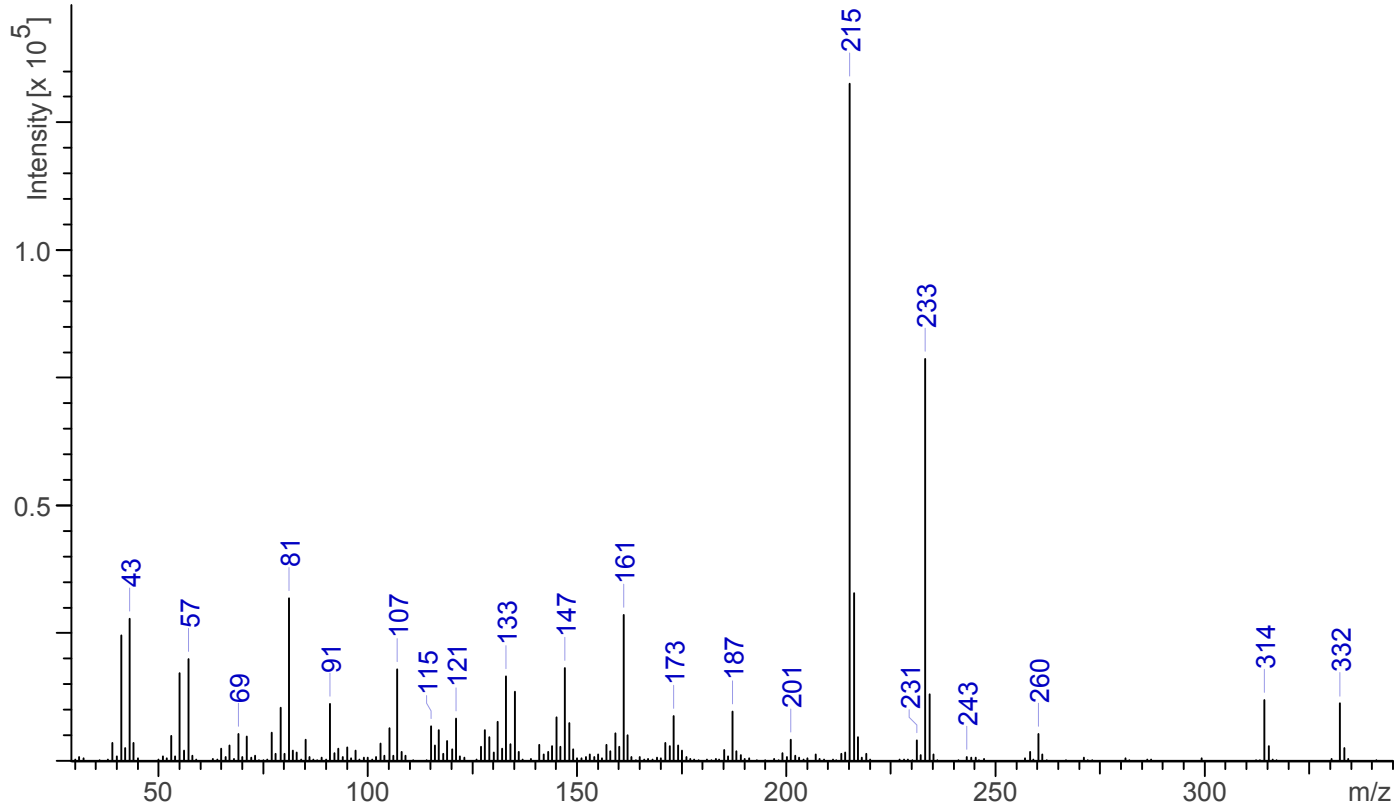


4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
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 = 20:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	16.864 min

EI Mass Spectrum: CP 47, 497-C8-homolog; Lot 0425163-4



4.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): CP 47,497-C8-homolog; Lot 0425163-4