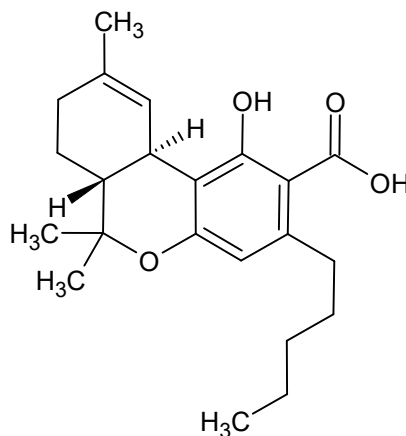




THCA-A

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



1. GENERAL INFORMATION

IUPAC Name: (6a*R*,10a*R*)-1-hydroxy-6,6,9-trimethyl-3-pentyl-6a,7,8,10a-tetrahydro-6*H*-benzo[*c*]chromene-2-carboxylic acid

CAS#: 23978-85-0

Synonyms: delta-9-tetrahydrocannabinolic acid, delta-9-THC carboxylic acid

Source: DEA Reference Material Collection

Appearance: Brown powder

UV_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
free acid	C ₂₂ H ₃₀ O ₄	358.47	Not Determined



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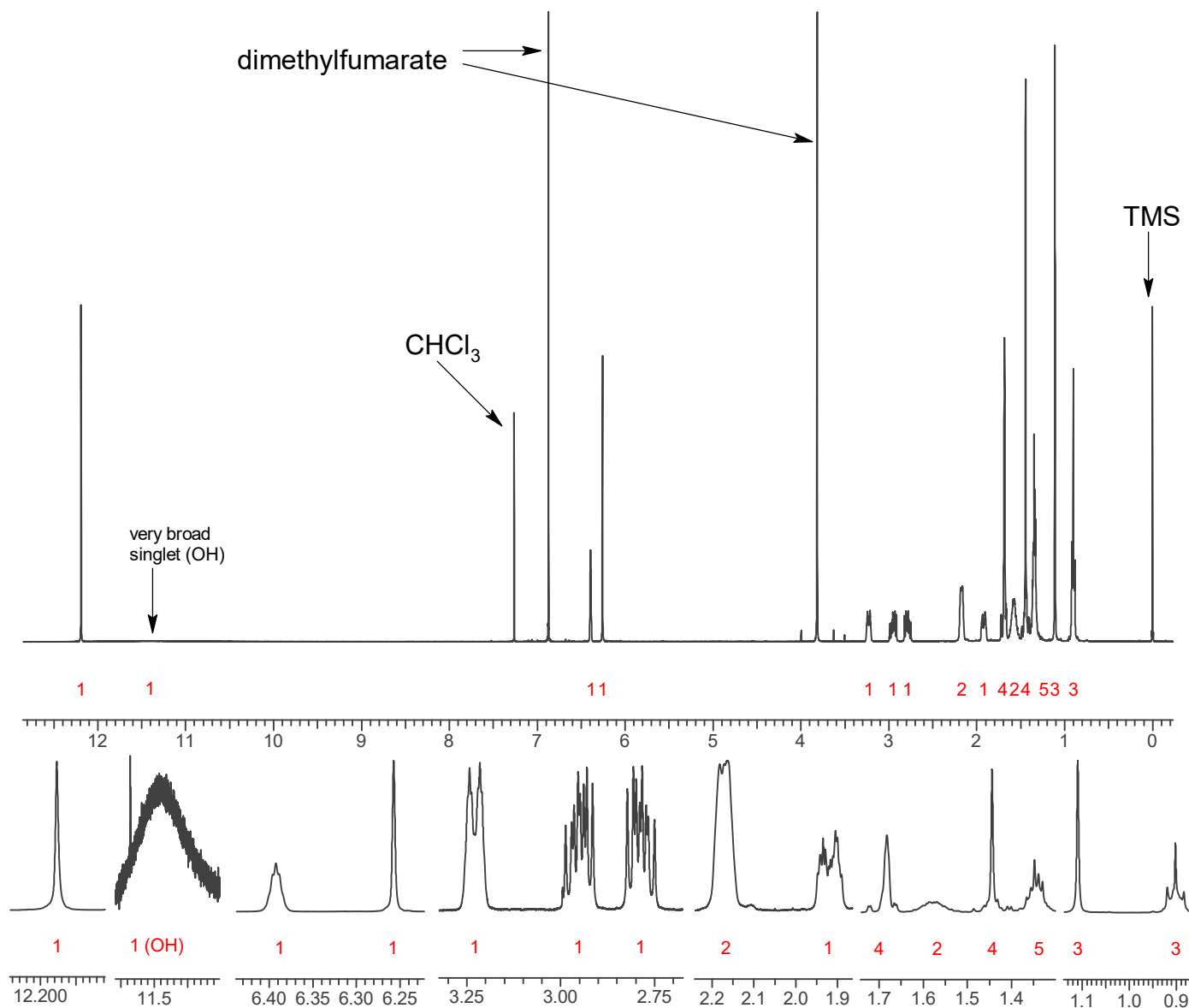
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 400MHzNMRspectrometer
Parameters: Spectralwidthatleastcontaining-3ppmthrough13ppm
Pulseangle90°
Delay between pulses: 45 seconds

¹HNMR: THCA-A; Lot 0477793-1; CDCl₃; 400MHz





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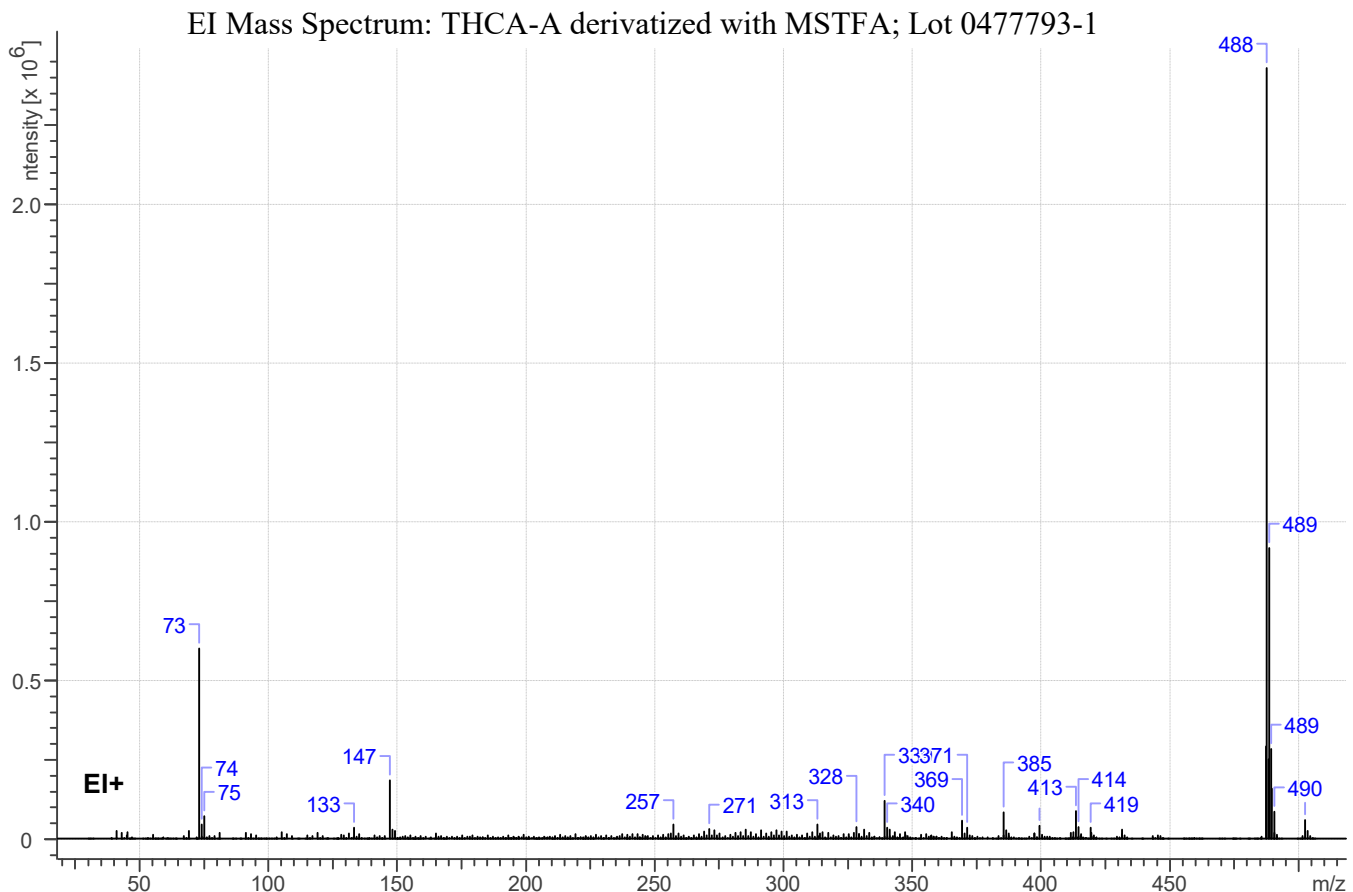


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃ derivatized with MSTFA.

Note: THCA-A not derivatized will convert to Δ⁹-THC.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5 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 280°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: 250
Tune file: stune.u Acquisition mode: scan
Retention Time: 16.253 min





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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 8
Number of background scans: 8
Resolution: 4 cm⁻¹
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): THCA-A; Lot 0477793-1

