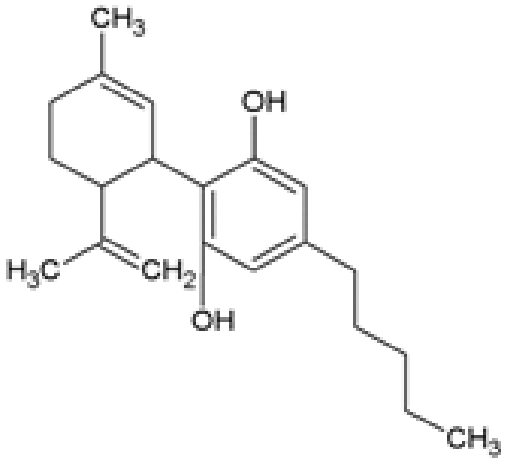
Cannabidiol

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



1. *GENERAL INFORMATION*

IUPAC Name:	2-[(1*R*,6*R*)-3-methyl-6-(prop-1-en-2-yl)cyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol
CAS#:	13956-29-1
Synonyms:	CBD
Source:	DEA Reference Material Collection
Appearance:	Yellow powder
UV_{max}(nm):	Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Neutral	$C_{21}H_{30}O_2$	314.46	68.02

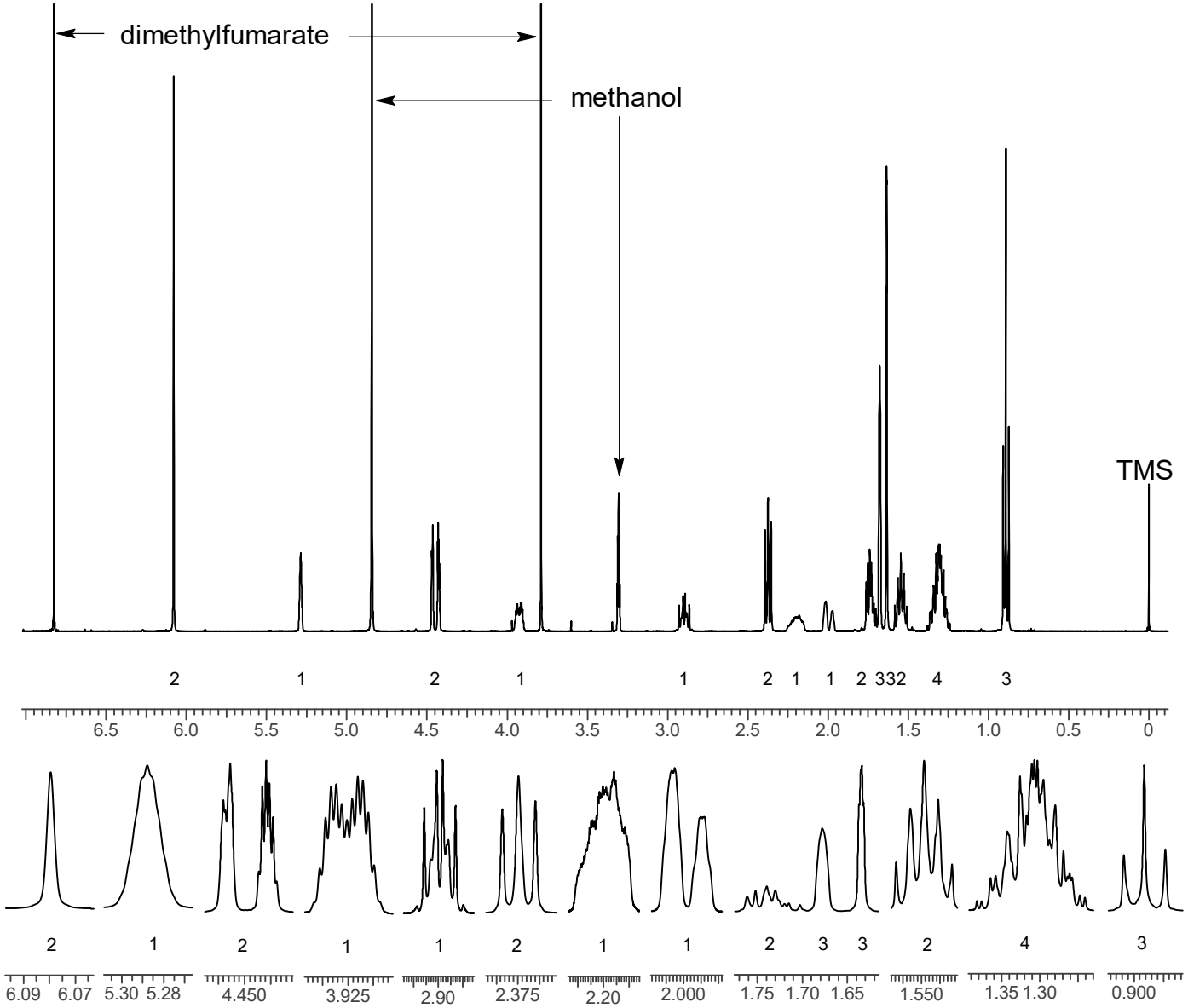
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~20 mg/mL in methanol-d_4 containing TMS for 0 ppm reference and dimethylfumarate 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

^{1}HNMR: Cannabidiol; Lot# 3857-52-1; methanol-d_4; 400MHz

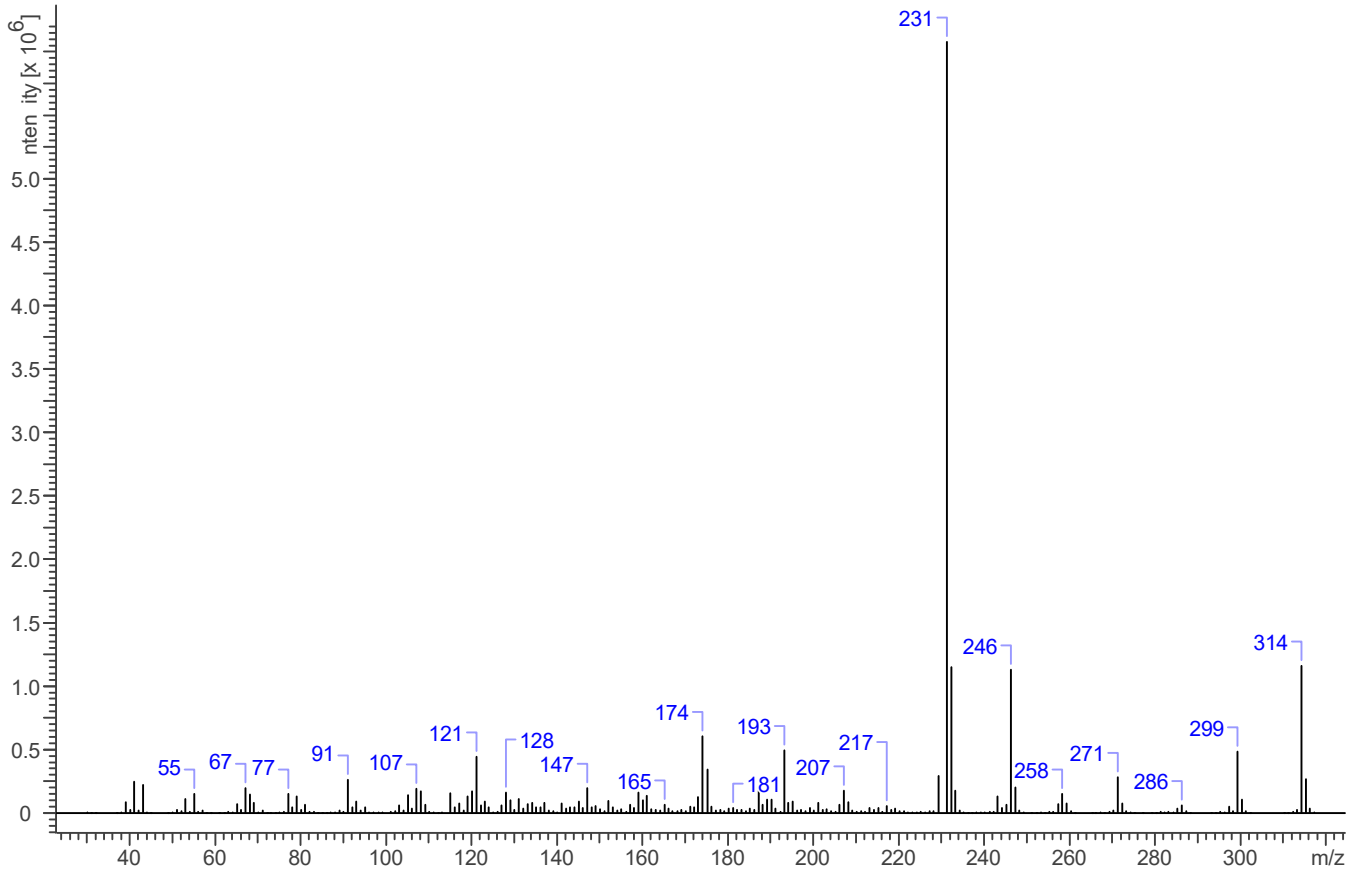


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in MeOH

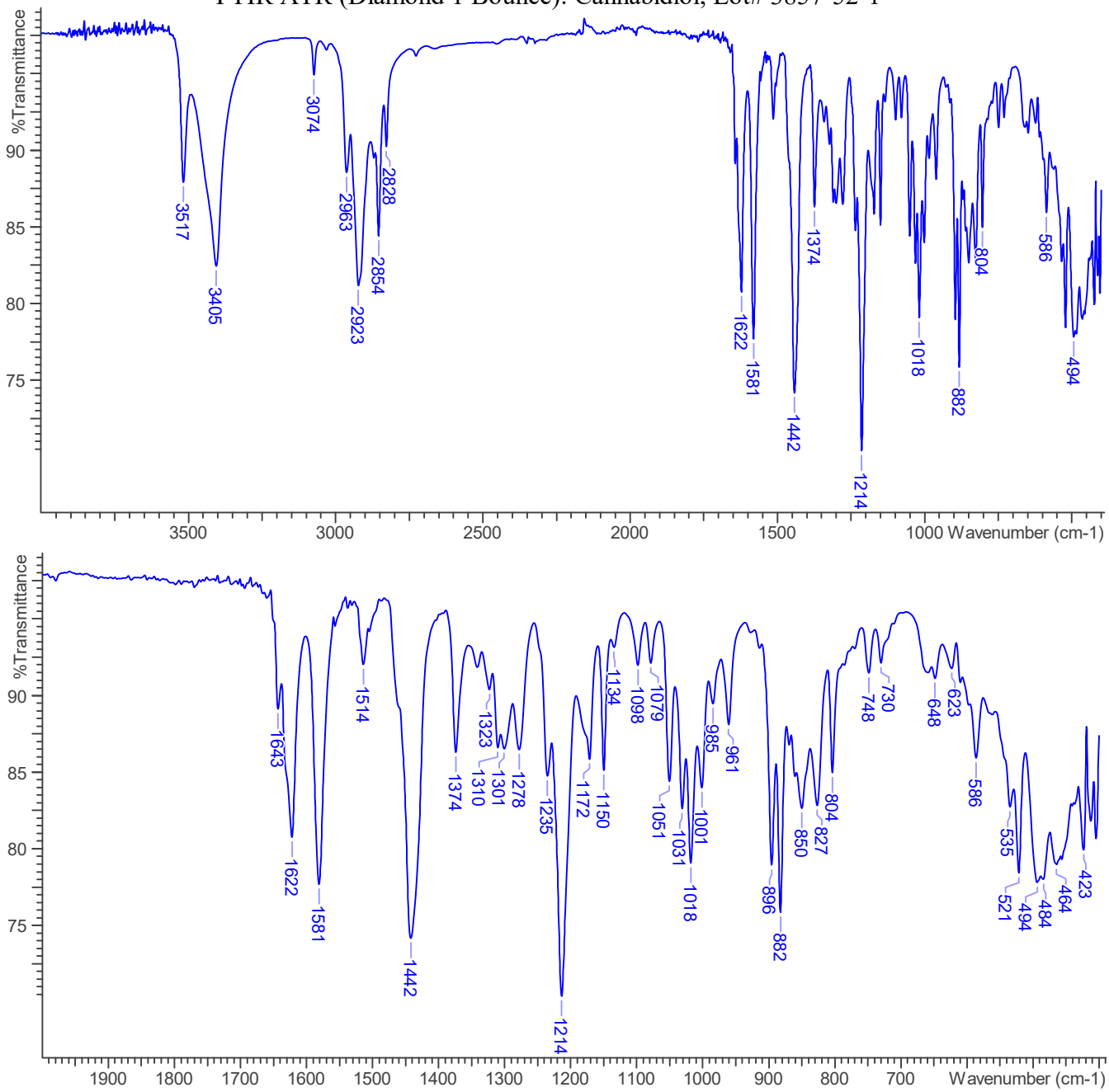
Instrument:	Agilent gas chromatograph operated in split mode with MS detector	
Column:	HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 µm	
Carrier Gas:	Helium at 1.5 mL/min	
Temperatures:	Injector: 280°C	MSD transfer line: 280°C
	MS Source: 230°C	MS Quad: 150°C
	Oven program:	
	1) 100°C initial temperature 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:	14.52 min	

EI Mass Spectrum: Cannabidiol; Lot# 3857-52-1



3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

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

FTIR ATR (Diamond 1 Bounce): Cannabidiol; Lot# 3857-52-1