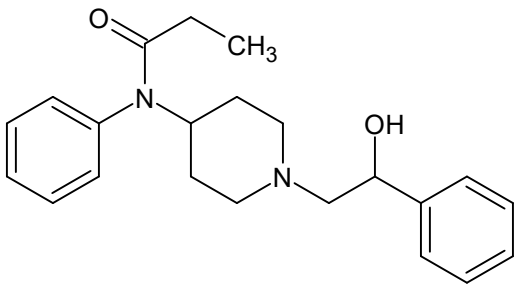
beta-Hydroxy fentanyl

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



1. GENERAL INFORMATION

IUPACName: *N*-(1-(2-hydroxy-2-phenylethyl)piperidin-4-yl)-*N*-phenylpropanamide

CAS#: 1473-95-6 (HCl)

Synonyms: N-[1-(2-hydroxy-2-phenethyl)-4-piperidinyl]-N-phenyl-propanamide, NIH 10506, R-4333, N-[1-(2-hydroxy-2-phenylethyl)piperidin-4-yl]-N-phenylpropanamide

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{22}H_{28}N_2O_2$	352.47	Not Determined
HCl	$C_{22}H_{28}N_2O_2$ HCl	388.93	Not Determined

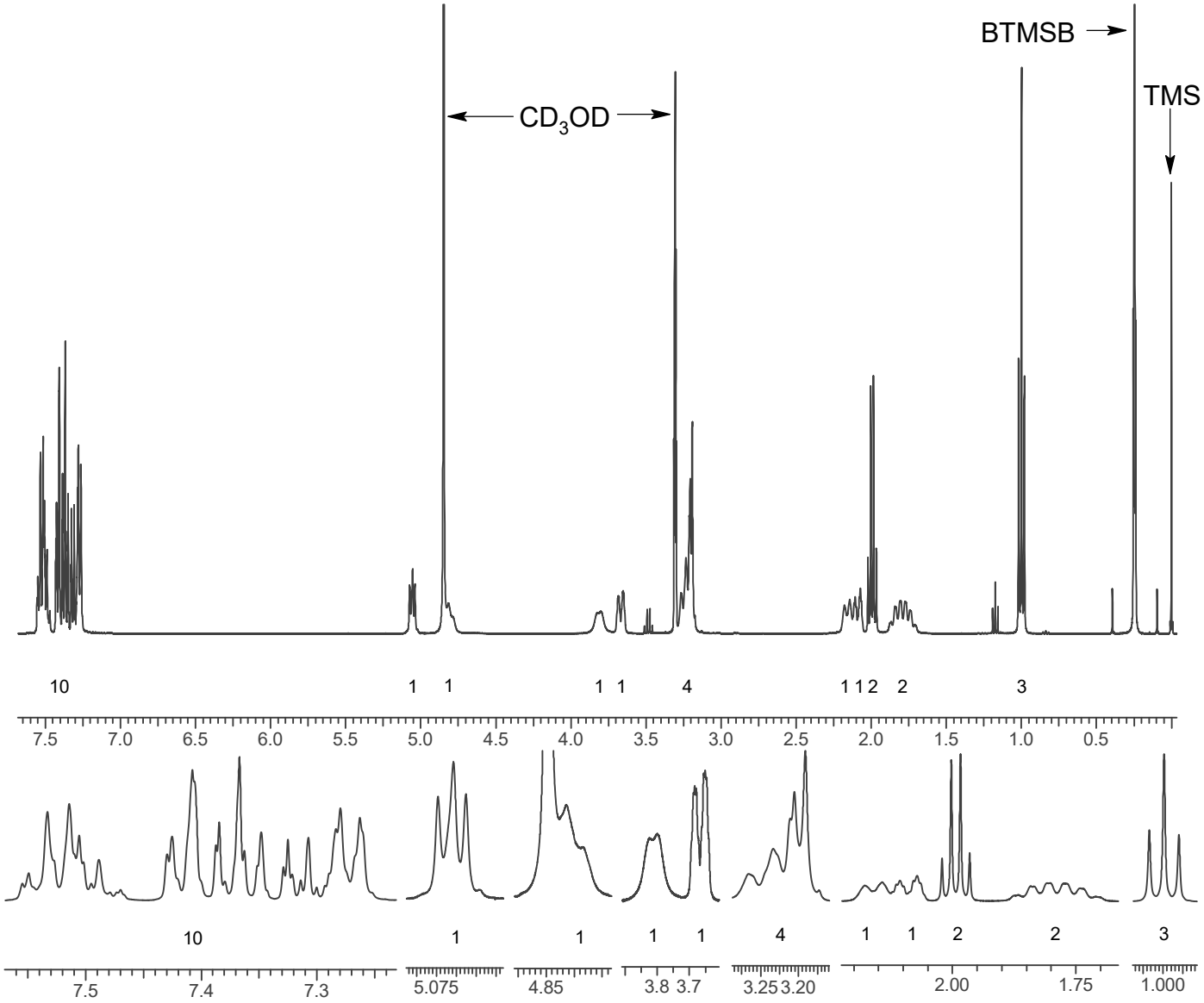
3. QUALITATIVEDATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in methanol-d_4 containing TMS for 0 ppm reference and 1,4-BTMSB-d_4 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: *beta*-Hydroxy fentanyl HCl; Lot # 0494095-19; CD_3OD; 400MHz

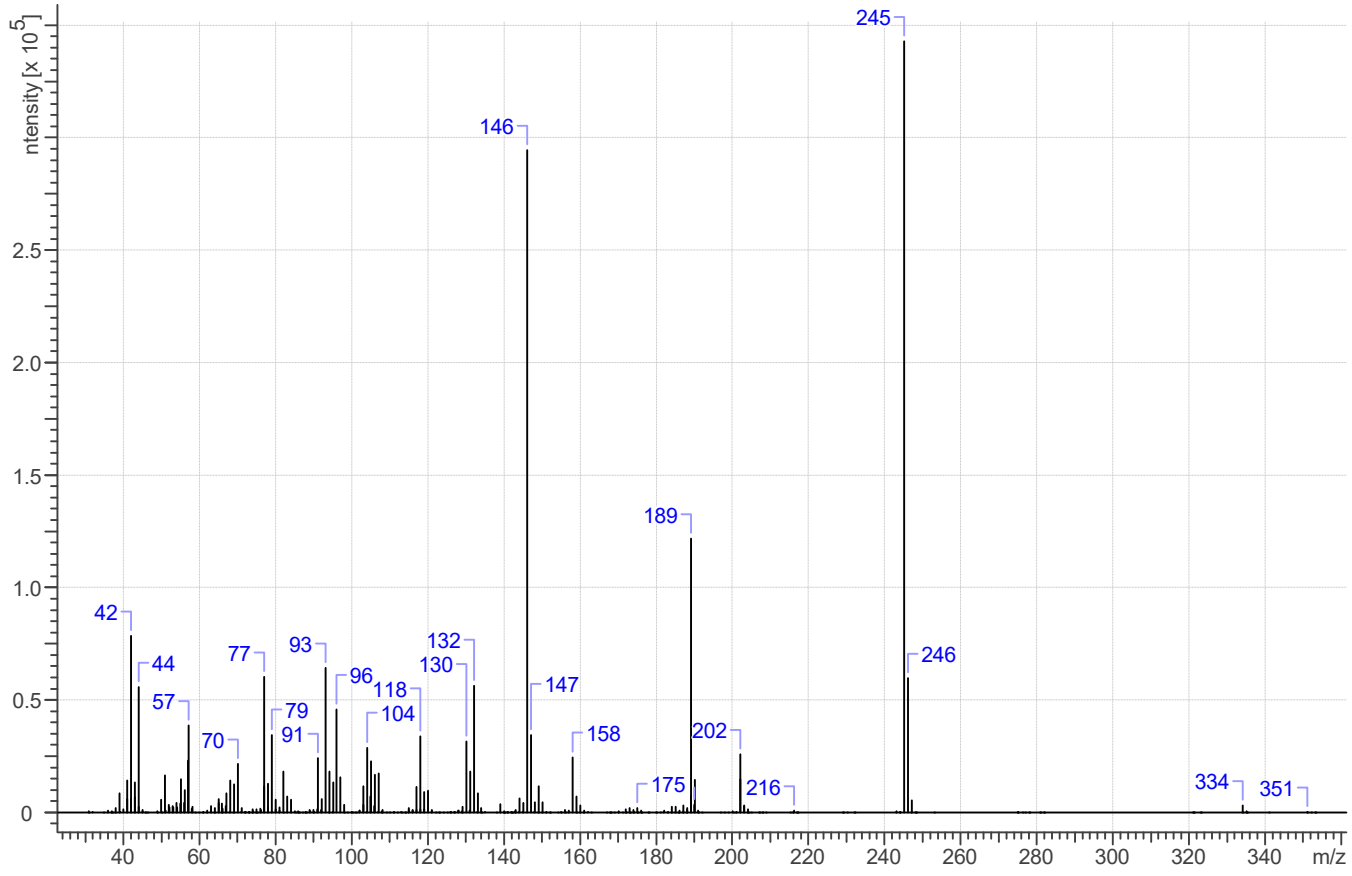


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

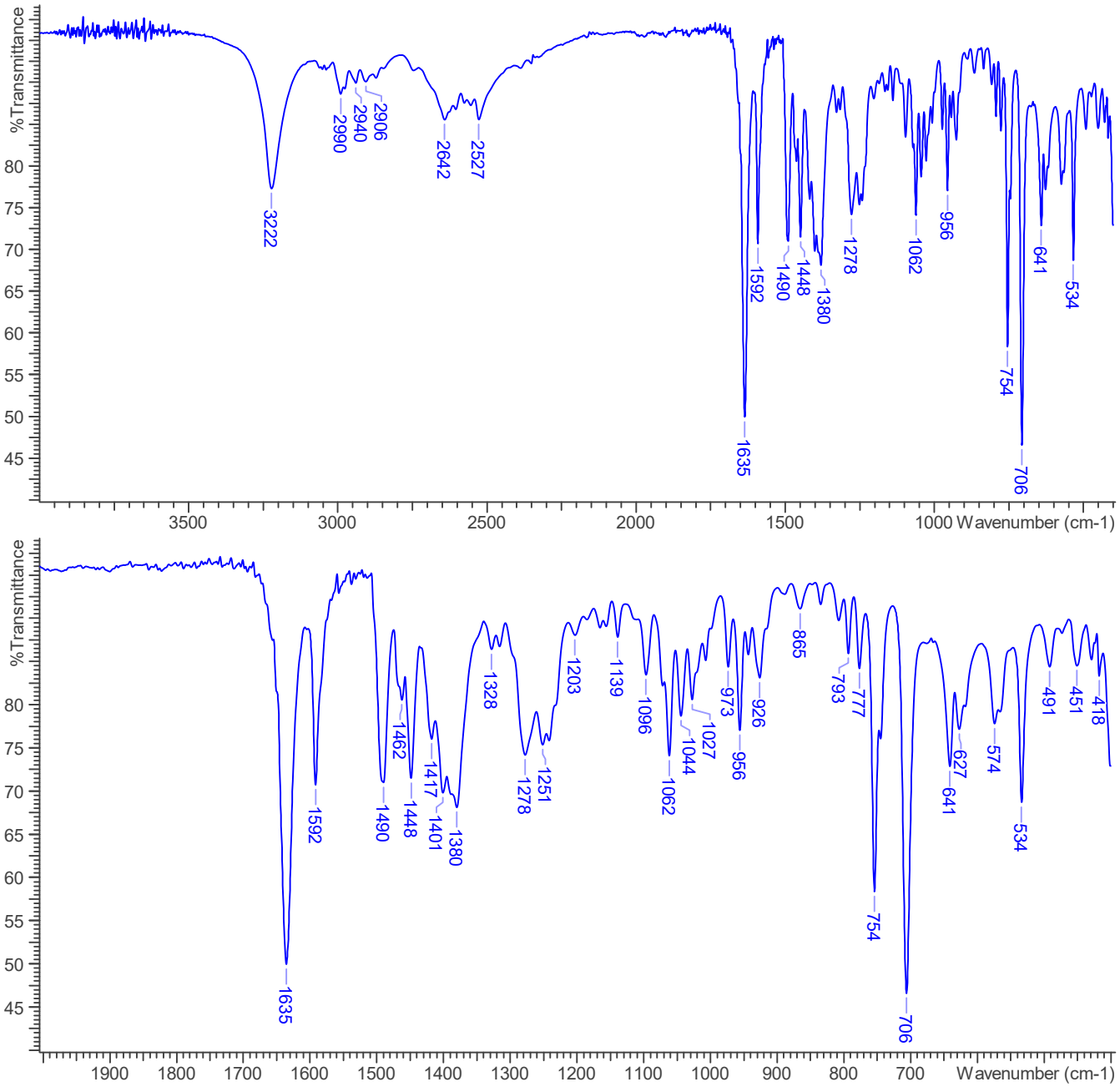
Instrument:	Agilent gas chromatograph operated in split mode with MS detector	
Column:	HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 µm	
Carrier Gas:	Helium at 1.5 mL/min	
Temperatures:	Injector: 280°C	MSD transfer line: 280°C
	MS Source: 230°C	MS Quad: 150°C
	Oven program:	
	1) 100°C initial temperature 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: 150
	Tune file: stune.u	Acquisition mode: scan
Retention Time:	18.528 min	

EI Mass Spectrum: *beta*-Hydroxy fentanyl HCl; Lot # 0494095-19



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): *beta*-Hydroxy fentanyl HCl; Lot # 0494095-19