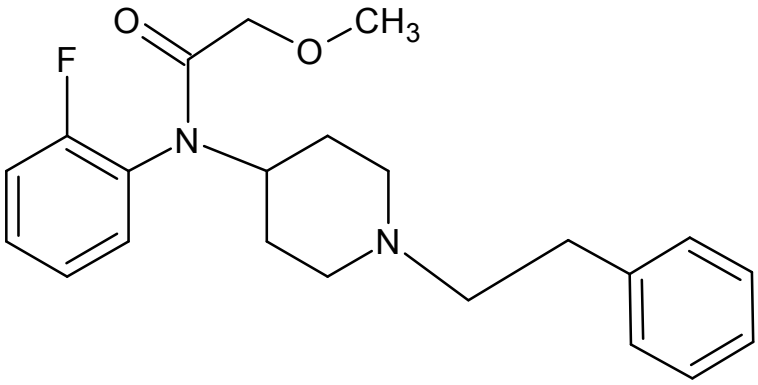
Ocfentanil

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



1. GENERAL INFORMATION

IUPAC Name: *N*-(2-fluorophenyl)-2-methoxy-*N*-(1-phenethylpiperidin-4-yl)acetamide

CAS#: 101343-69-5

Synonyms: Ocfentanyl;
N-(2-fluorophenyl)-2-methoxy-N-[1-(2-phenylethyl)piperidin-4-yl]acetamide

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{22}H_{27}FN_2O_2$	370.46	Not Determined
HCl	$C_{22}H_{27}FN_2O_2 \cdot HCl$	406.92	Not Determined

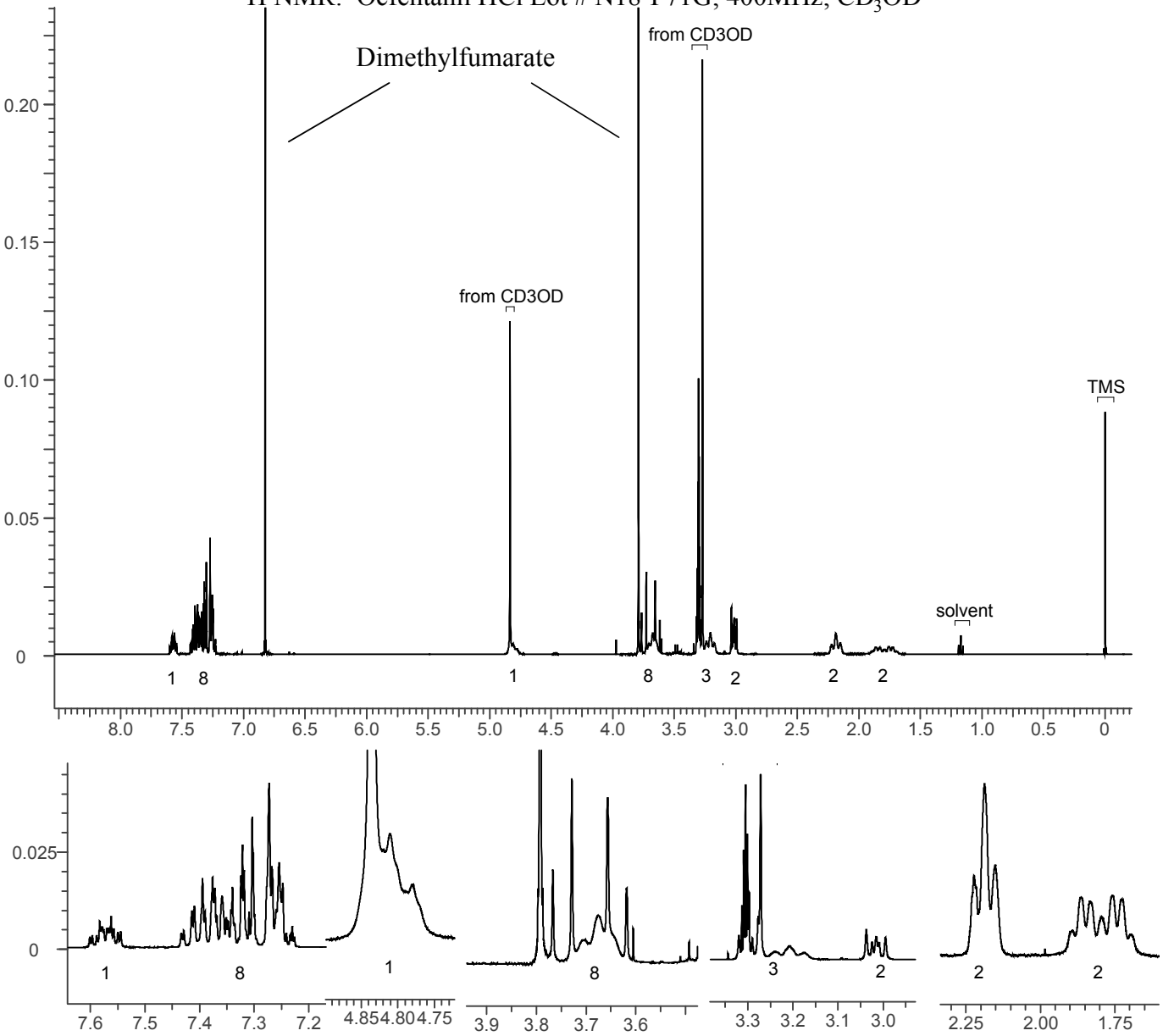
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in CD_3OD 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}H NMR: Ocfentanil HCl Lot # N18-P71G; 400MHz; CD_3OD

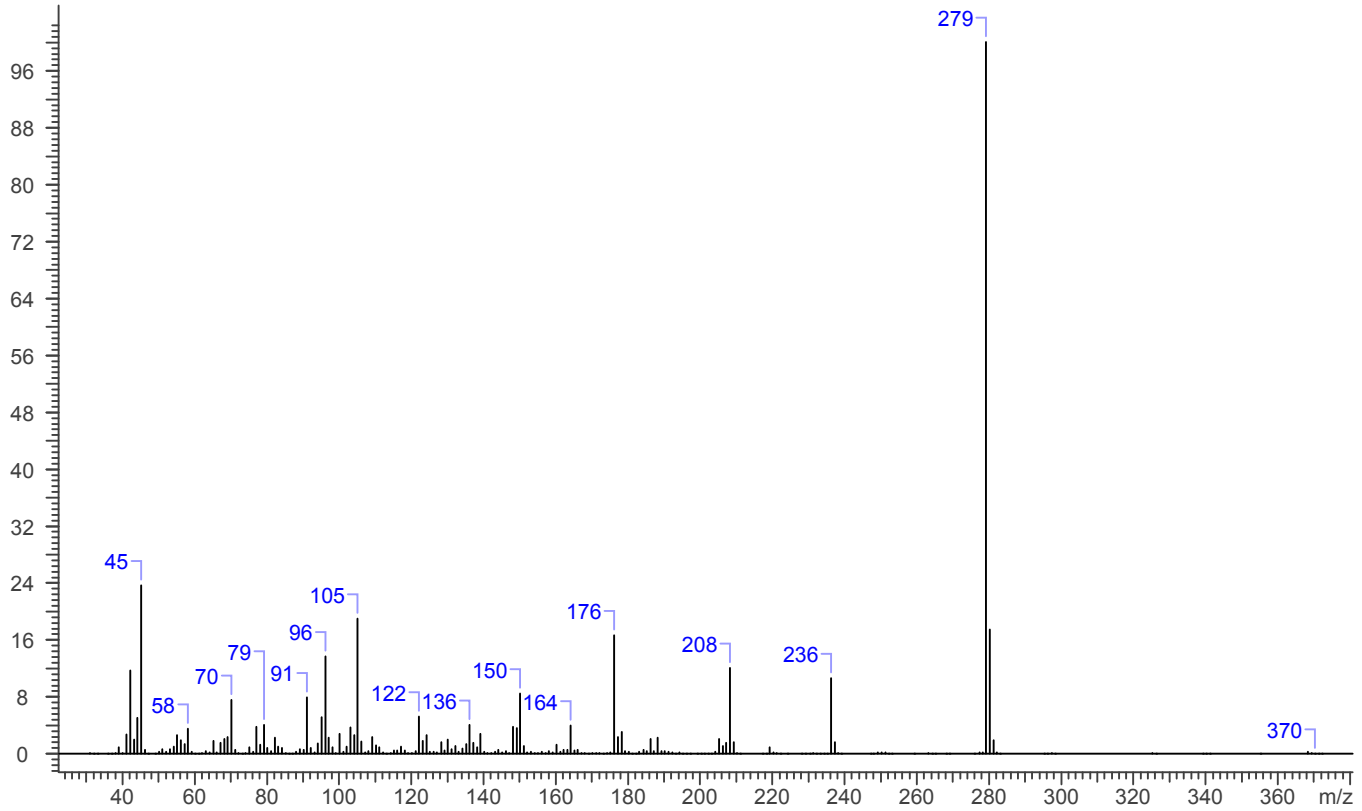


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in 9:1 chloroform:methanol.

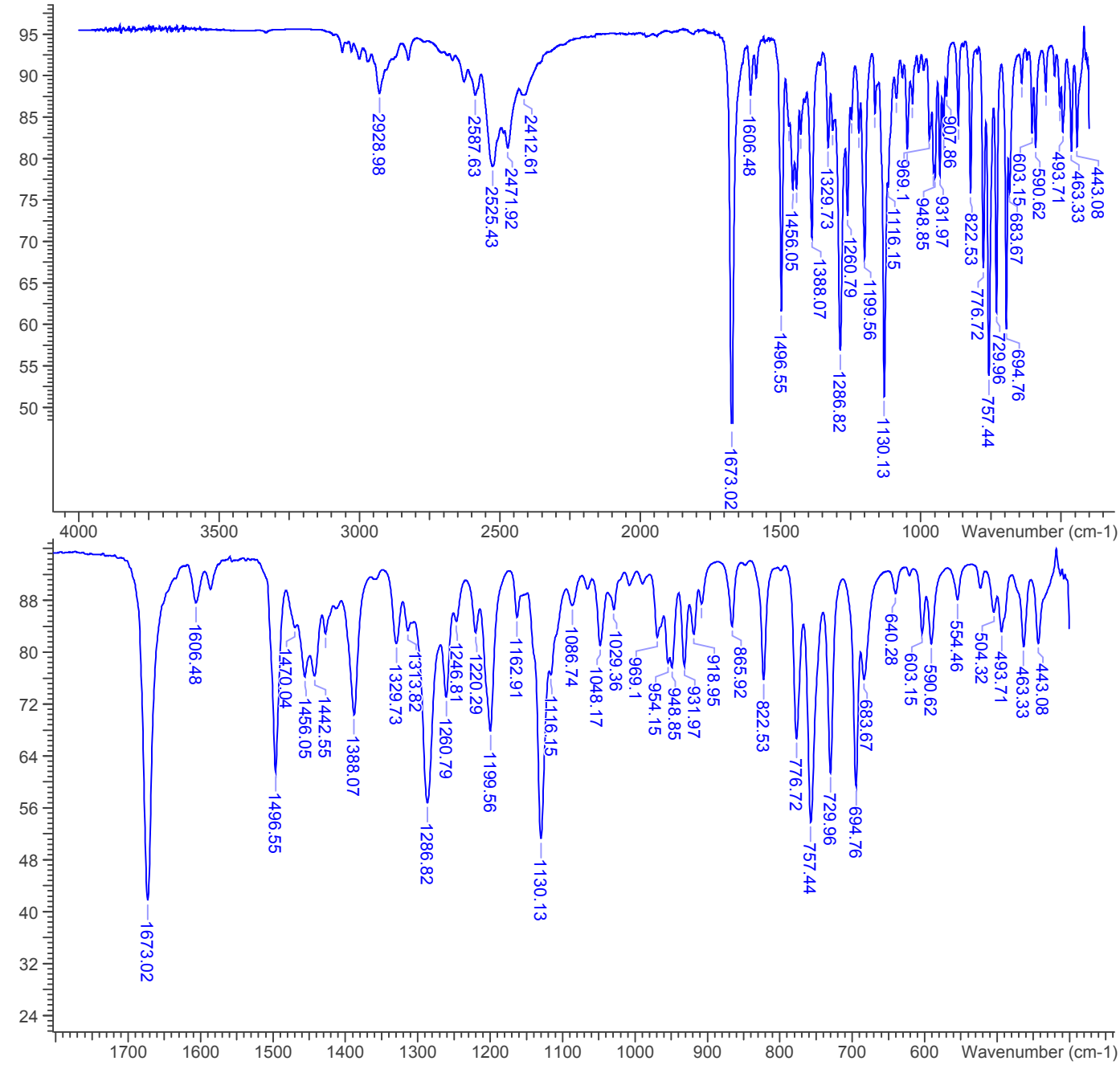
Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 m
Carrier Gas:	Helium at 1.5 mL/min
Temperatures:	Injector: 280°C
	MSD transfer line: 280°C
	MS Source: 230°C
	MS Quad: 150°C
	Oven program:
	1) 100°C initial temperature 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 L injected
MS Parameters:	Mass scan range: 30-550 amu
	Threshold: 250
	Tune file: stune.u
	Acquisition mode: scan
Retention Time:	17.515 min

EI Mass Spectrum: Ocfentanil HCl Lot # N18-P71G



3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 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): Ocfentanil HCl Lot # N18-P71G