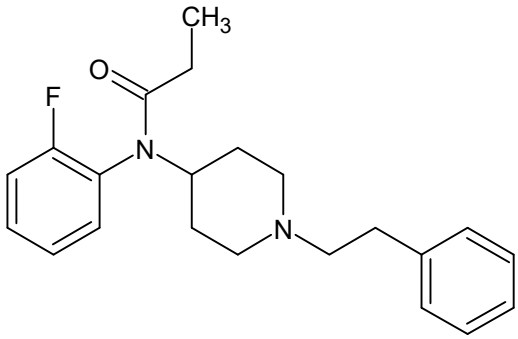
ortho-Fluorofentanyl

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)-*N*-[1-(2-phenylethyl)-4-piperidinyl]propanamide

CAS#: N/A

Synonyms: o-fluorofentanyl, 2-fluorofentanyl, ortho-F-fentanyl

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	$C_{22}H_{27}FN_2O$	354.46	Not Determined
HCl	$C_{22}H_{27}FN_2O$ HCl	390.92	233.5

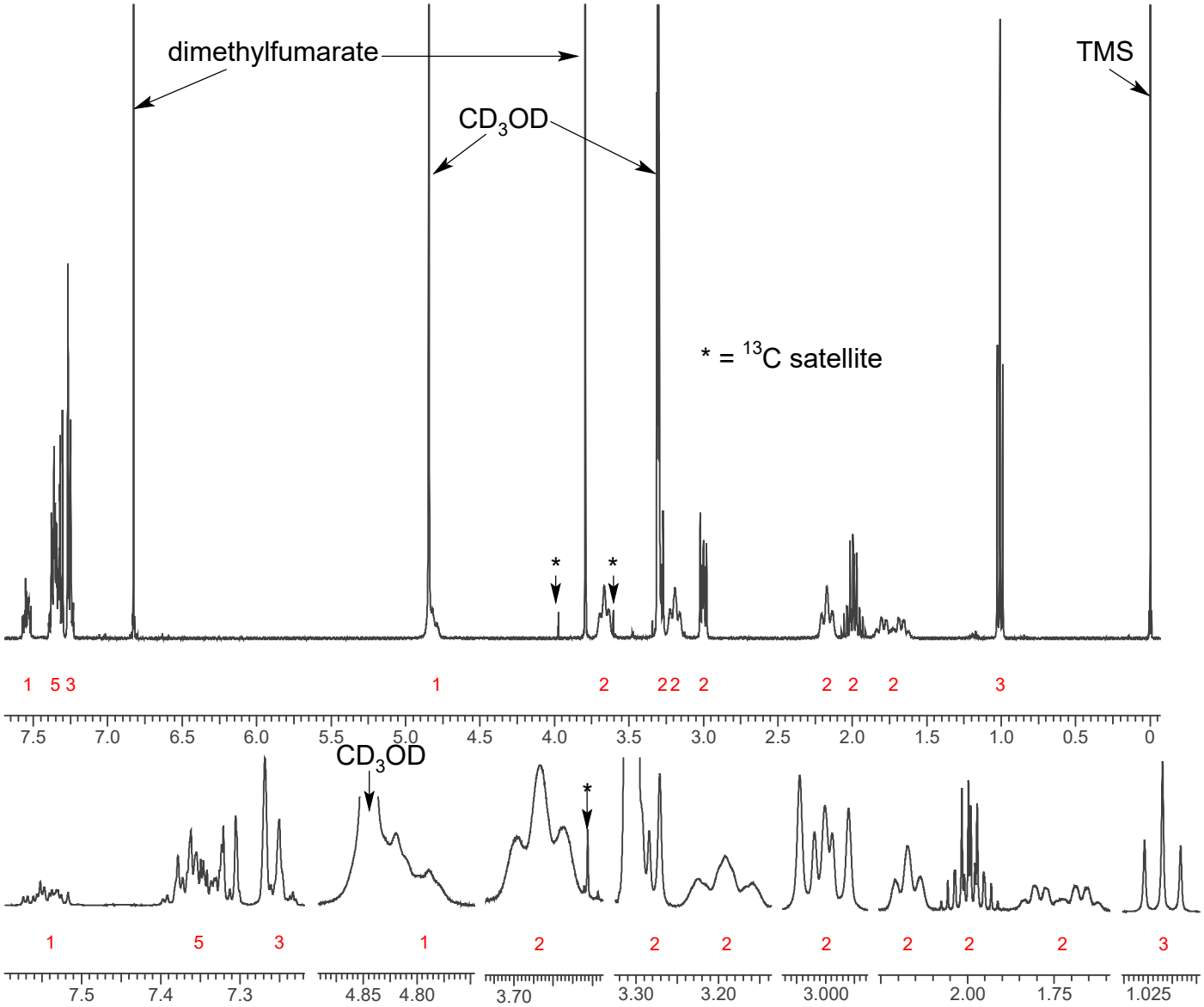
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 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}HNMR: ortho-Fluorofentanyl HCl; LOT # RM-160713-01; CD_3OD; 400MHz

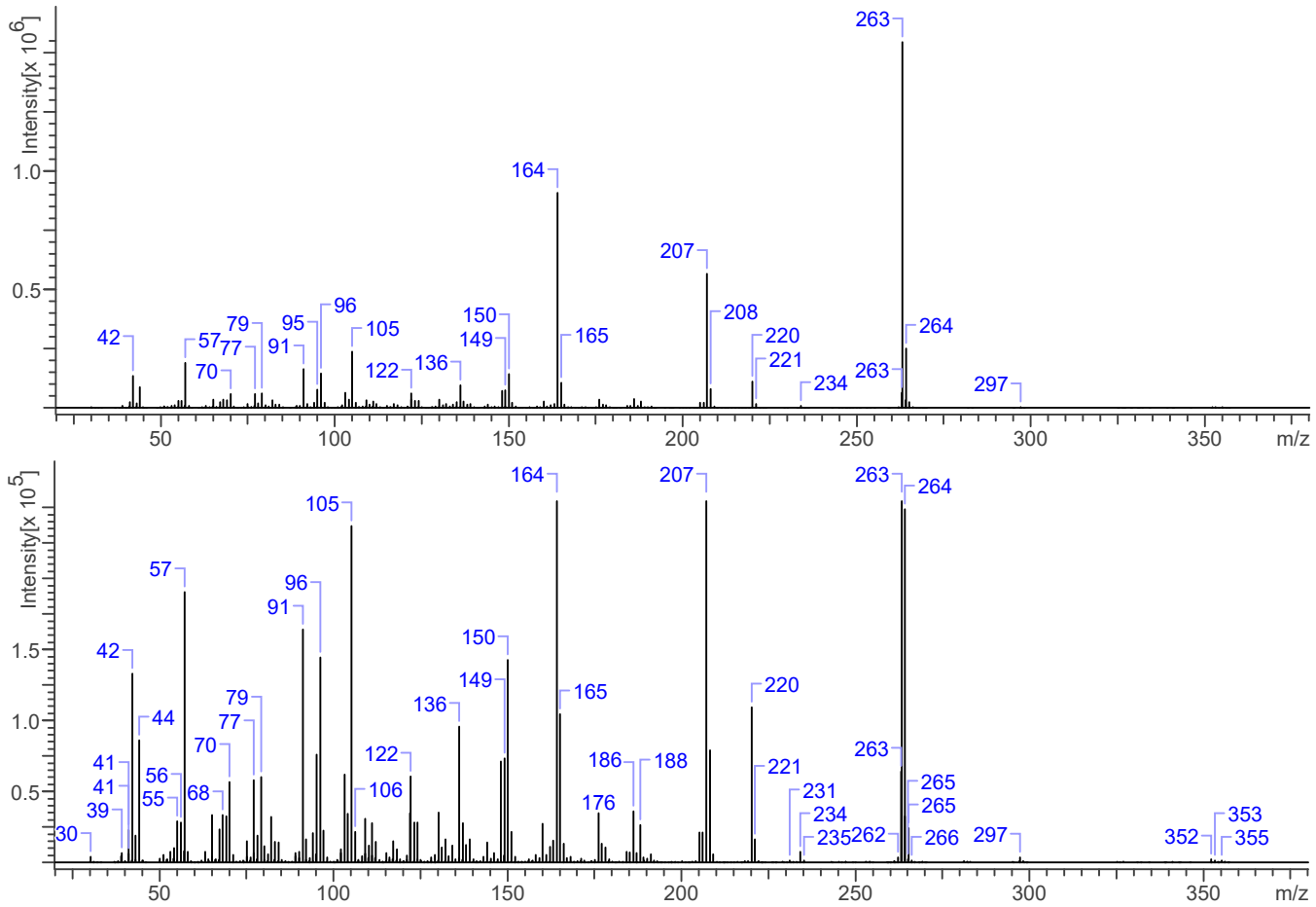


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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:	16.885 min

EI Mass Spectrum: ortho-Fluorofentanyl HCl; LOT # RM-160713-01

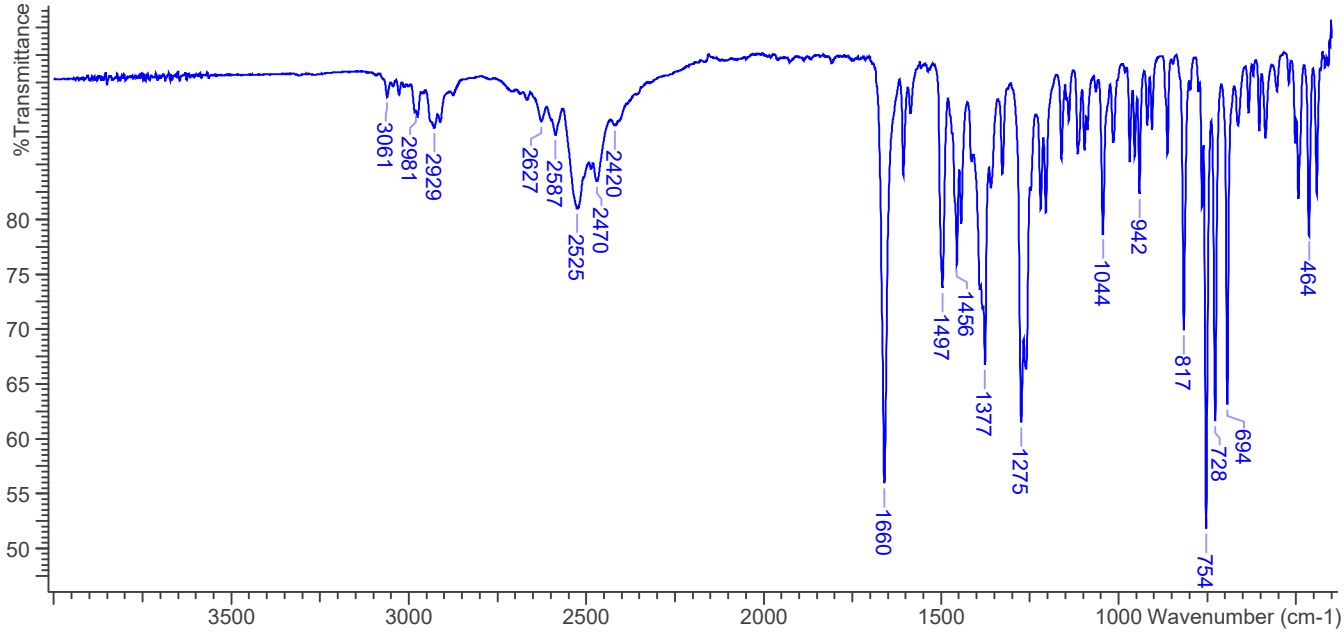


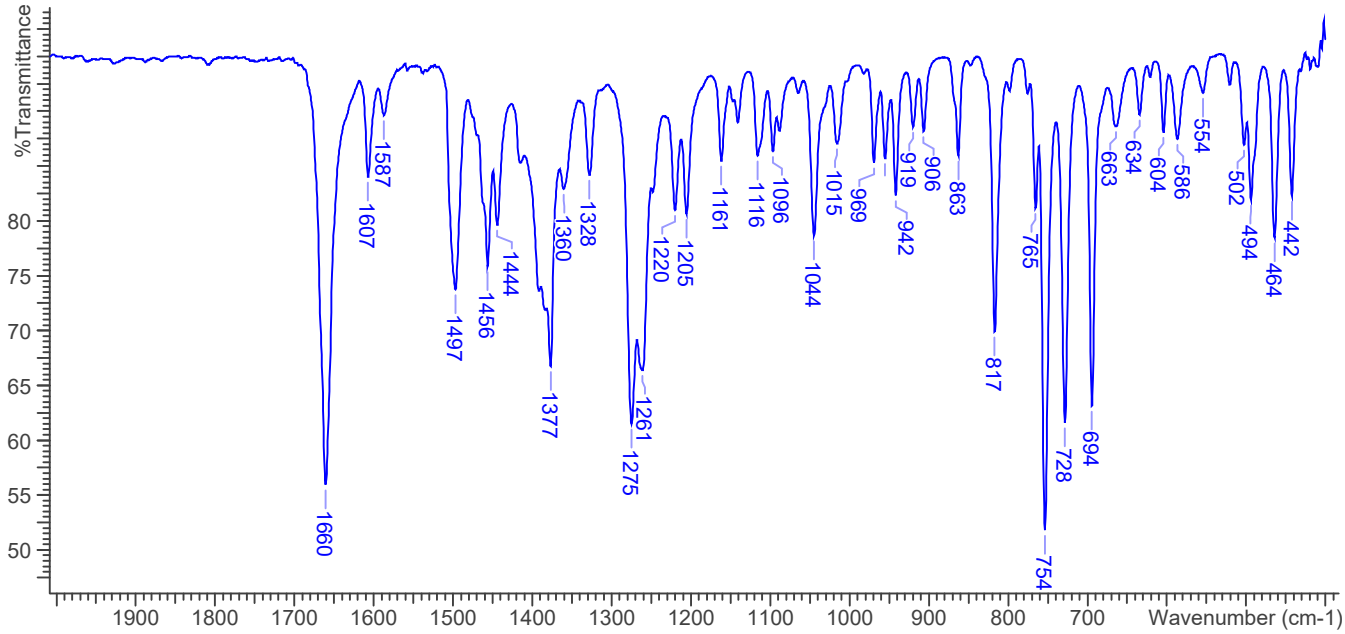
3.3 INFRARED SPECTROSCOPY (FTIR)

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: 4
Aperture: 80

FTIR ATR (Diamond 1 Bounce): ortho-Fluorofentanyl HCl; LOT # RM-160713-01





4. ADDITIONAL RESOURCES

No additional resources as of 09/2016