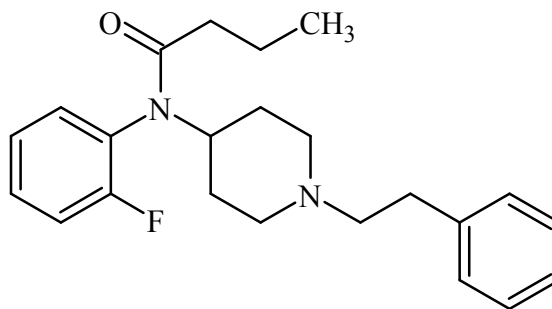




ortho-Fluorobutyryl fentanyl

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)piperidin-4-yl]butanamide

CAS#: NA

Synonyms: 2-FBF, o-FBF, 2-Fluorobutyryl fentanyl, o-Fluorobutyryl fentanyl

Source: DEA Reference Material Collection

Appearance: white powder

UV_{max}(nm): NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₂₉ N ₂ O	368.49	Not Determined
HCl	C ₂₃ H ₂₉ N ₂ O HCl	404.95	Not Determined



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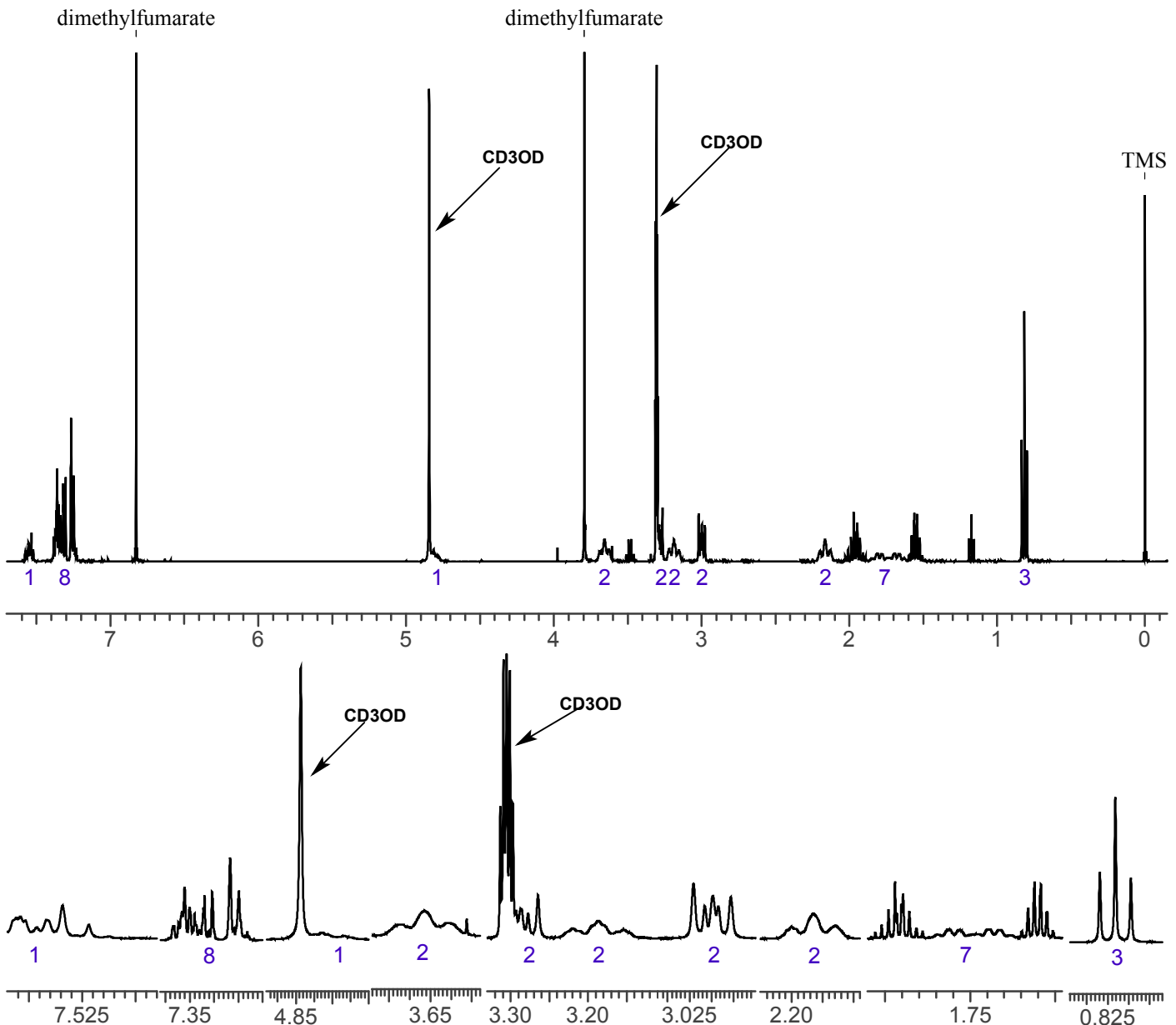
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6mg/mL in CD₃OD 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

¹HNMR: ortho-Fluorobutyryl fentanyl HCl Lot# 0513603-3; CD₃OD; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5; 30m x 0.25 mm x 0.25 μ 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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

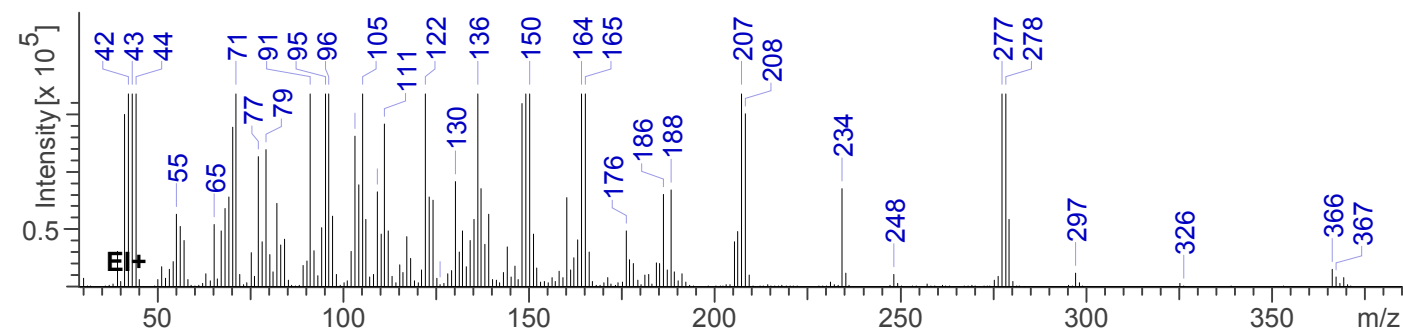
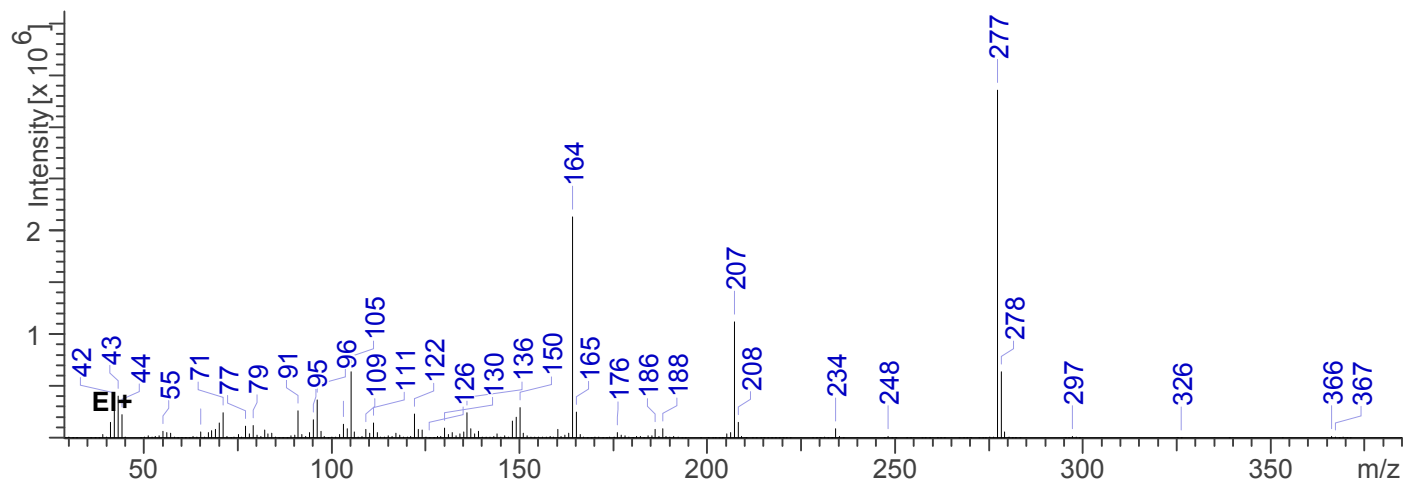
Threshold: 250

Tune file: stune.u

Acquisition mode: scan

Retention Time: 17.281 min

EI Mass Spectrum: ortho-Fluorobutyryl fentanyl HCl Lot# 0513603-3





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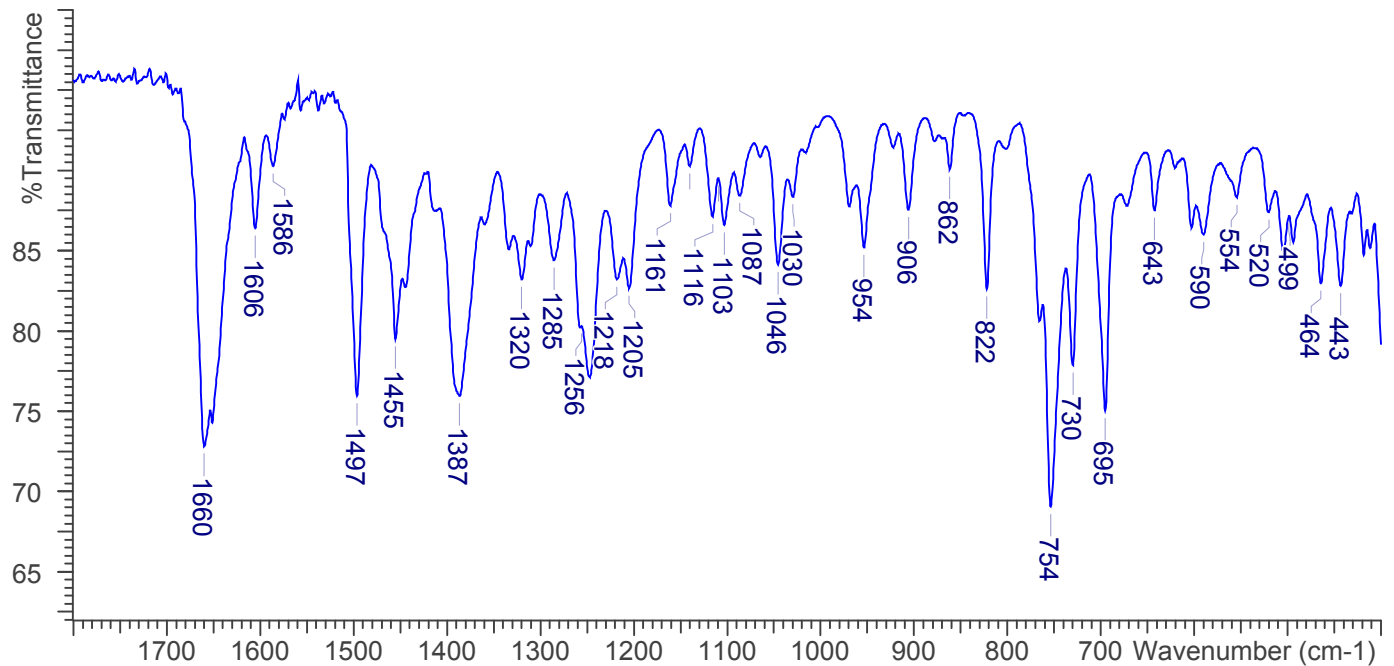
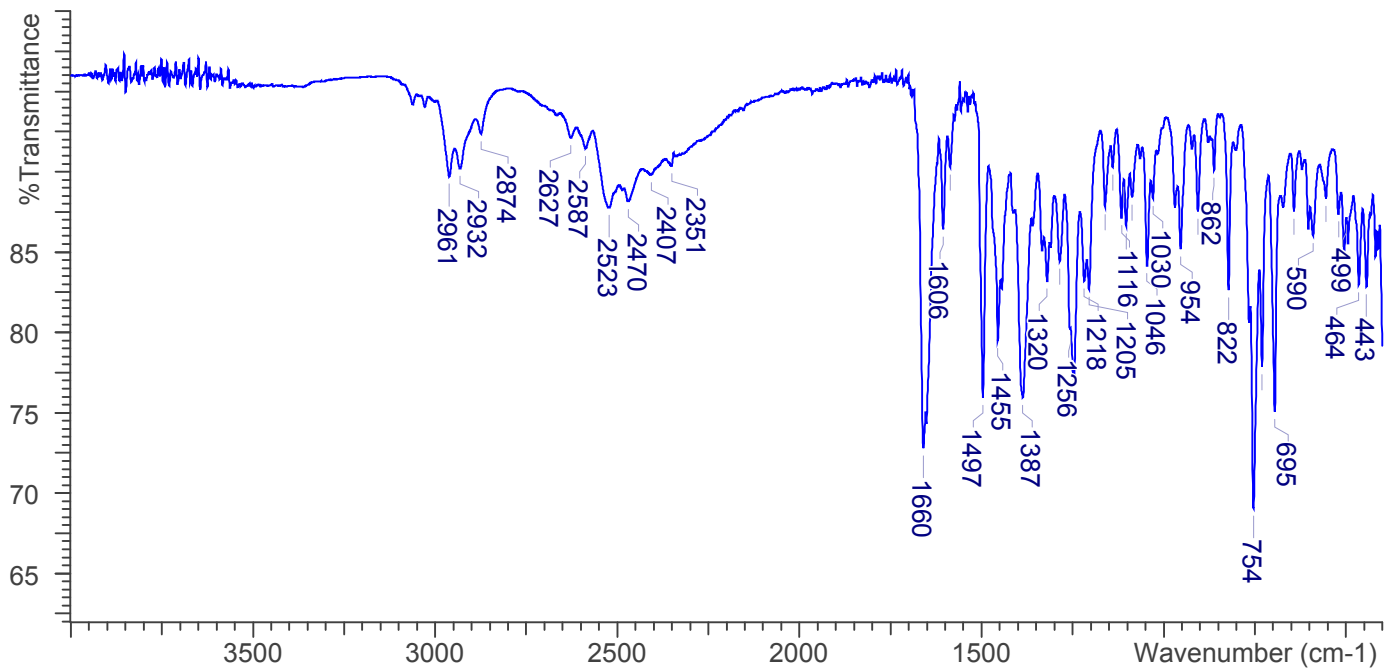


3.3 INFRARED SPECTROSCOPY (FTIR)

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): ortho-Fluorobutyryl fentanyl HCl Lot# 0513603-3





ortho-Fluorobutyryl fentanyl

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4. ADDITIONAL RESOURCES

No available literature as of 04/06/18