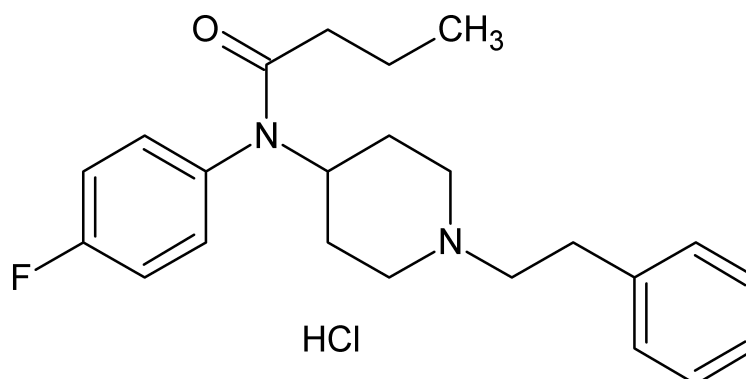




para-fluorobutyryl fentanyl

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



1. GENERAL INFORMATION

IUPAC Name: N-(4-fluorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]butanamide

CAS#: 244195-31-1

Synonyms: p-FBF, p-fluorobutyryl 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 (°C)
Base	C ₂₃ H ₂₉ FN ₂ O	368.48	Not Determined
HCl	C ₂₃ H ₂₉ FN ₂ O · HCl	404.94	Not Determined



para-fluorobutyryl fentanyl

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



3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in DMSO containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

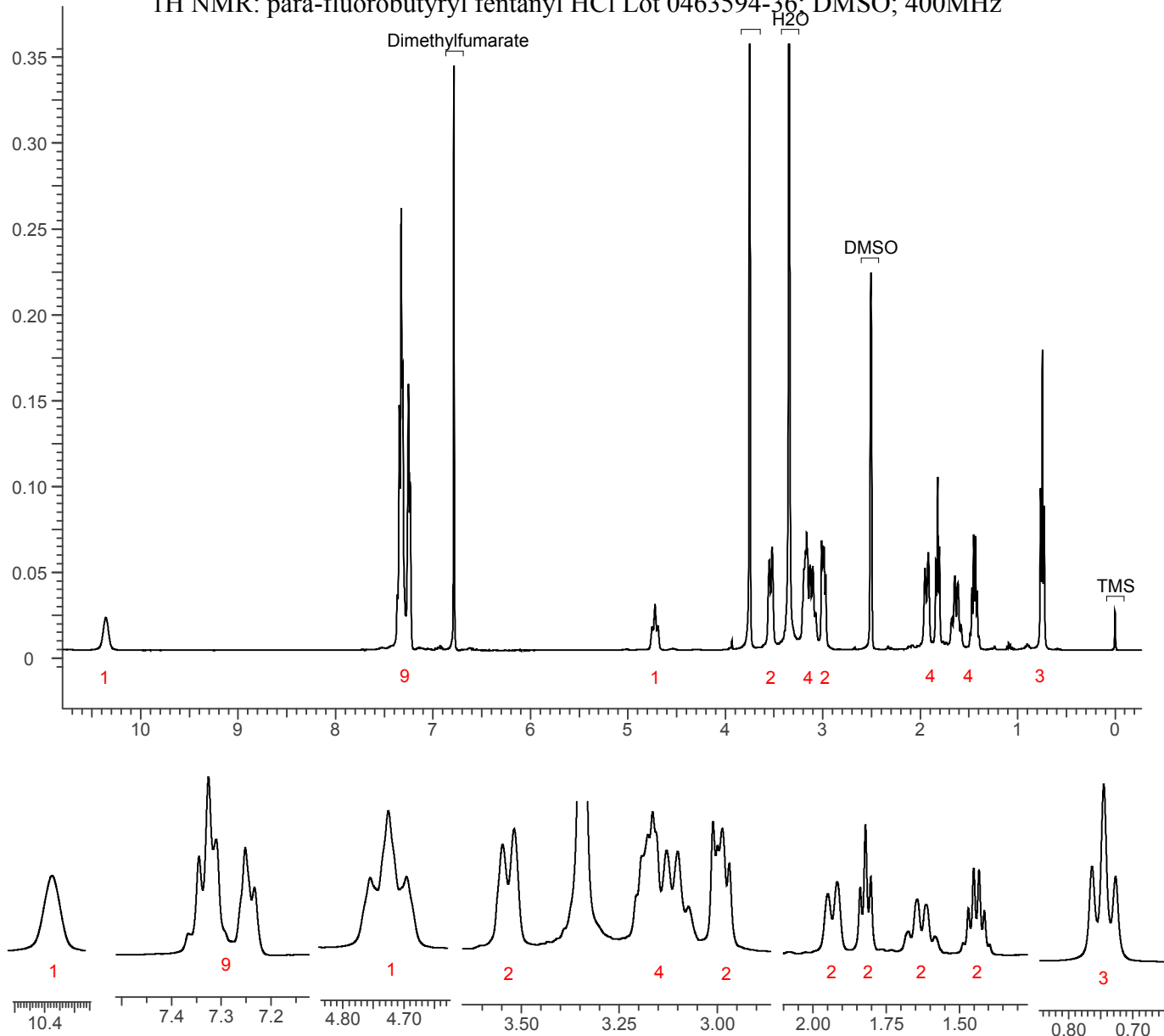
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: para-fluorobutyryl fentanyl HCl Lot 0463594-36; DMSO; 400MHz





para-fluorobutyryl fentanyl

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

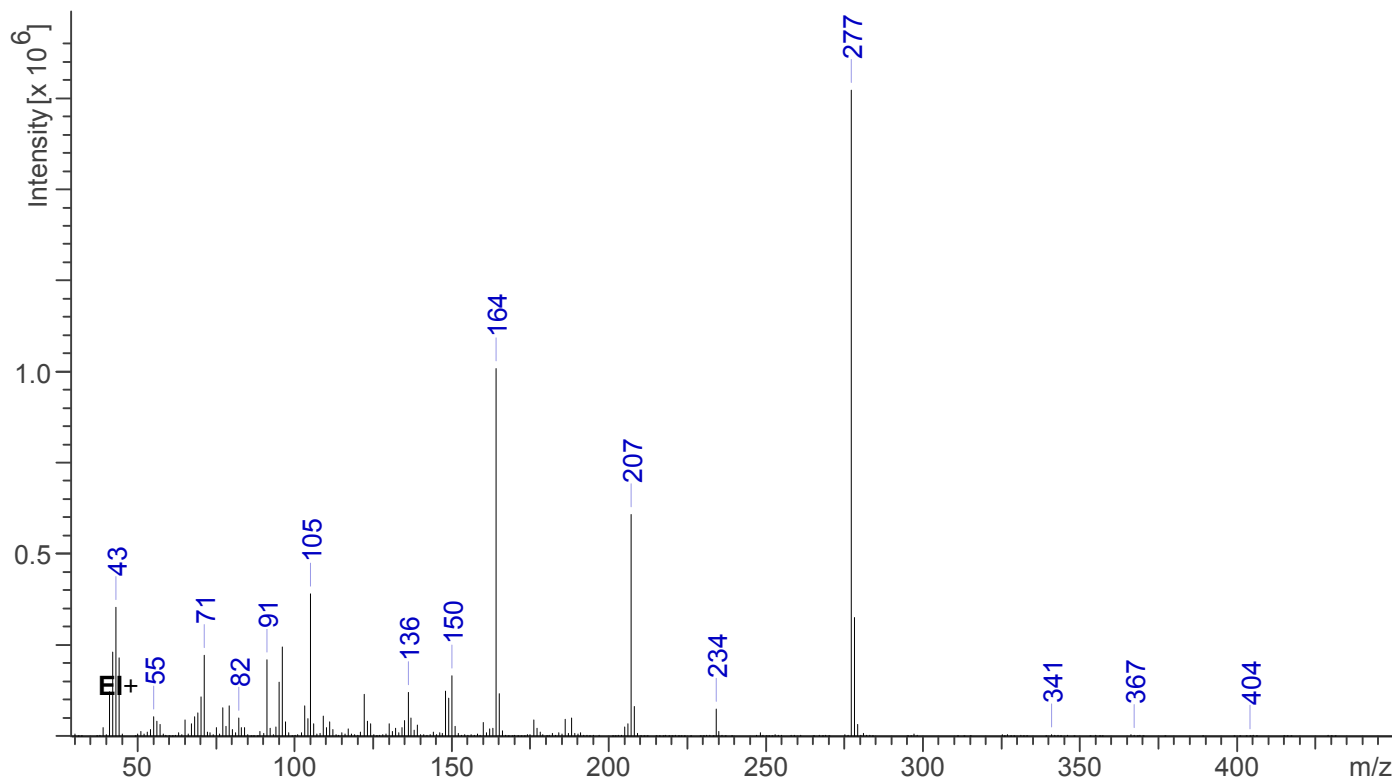


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~2mg/mL MeOH.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-5 MS (or equivalent); 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: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 17.292 min

EI Mass Spectrum: para-fluorobutyryl fentanyl HCl Lot 0463594-36





para-fluorobutyryl fentanyl

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

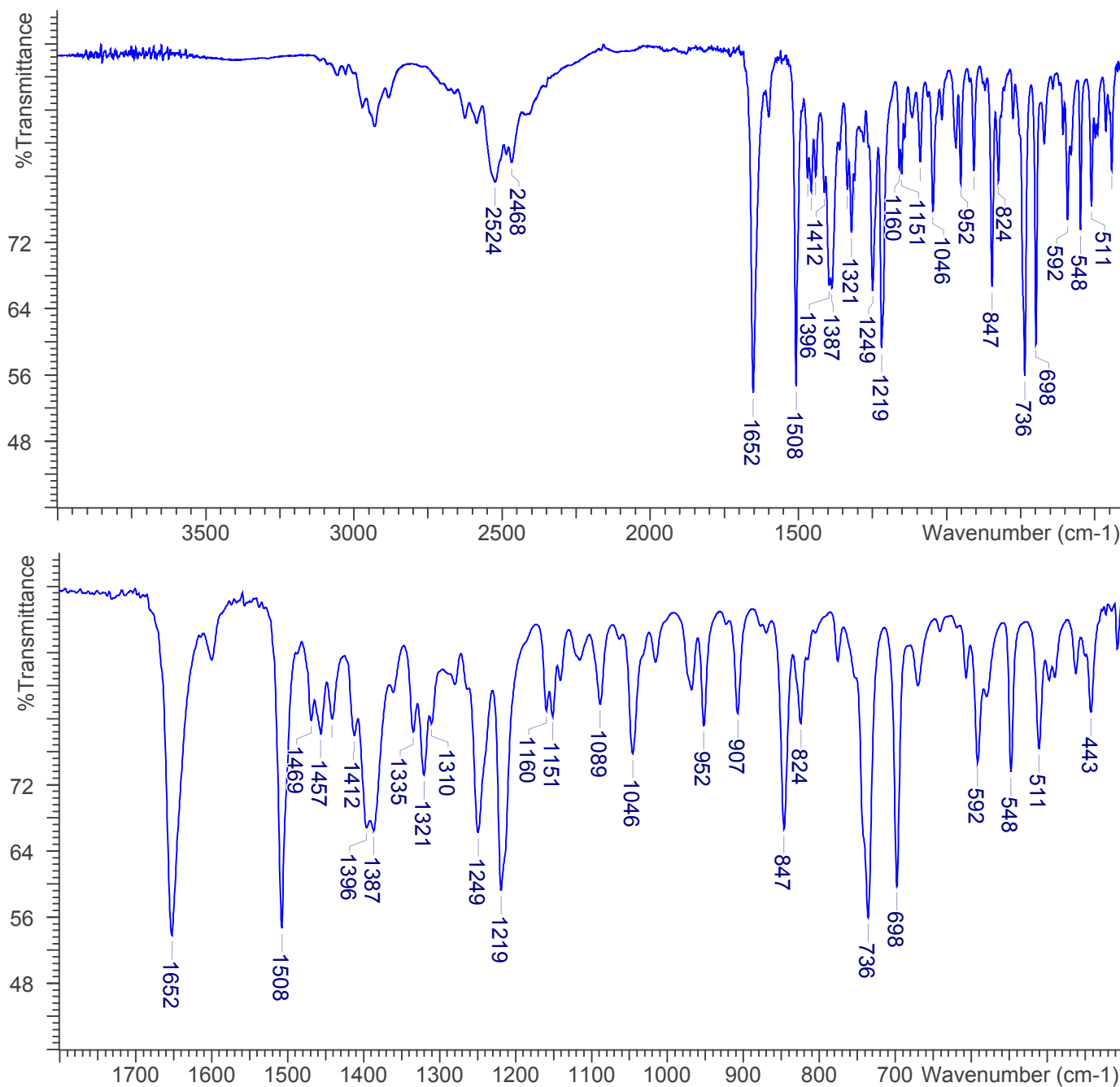


3.3 INFRARED SPECTROSCOPY (FTIR)

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): para-Fluorobutyryl fentanyl HCl; Lot 0463594-36





para-fluorobutyryl fentanyl

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



4. ADDITIONAL RESOURCES

[Wikipedia](#)