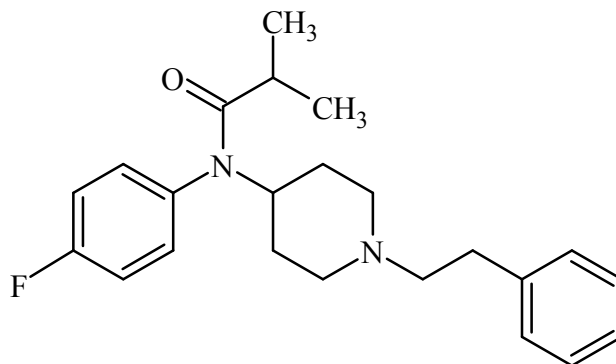




## 4-Fluoroisobutyrylfentanyl

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	<i>N</i> -(4-fluorophenyl)- <i>N</i> -(1-phenethylpiperidin-4-yl)isobutyramide
<b>CAS#:</b>	NA
<b>Synonyms:</b>	<i>p</i> -fluoroisobutyryl fentanyl, para-fluoroisobutyryl fentanyl, <i>N</i> -(4-fluorophenyl)-2-methyl- <i>N</i> -[1-(2-phenethyl)piperidin-4-yl]propanamide
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	white powder (HCl)
<b>UV<sub>max</sub>(nm):</b>	NA

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>23</sub> H <sub>29</sub> FN <sub>2</sub> O	368.48	NA
HCl	C <sub>23</sub> H <sub>29</sub> FN <sub>2</sub> O · HCl	404.95	NA



# 4-Fluoroisobutyrylfentanyl

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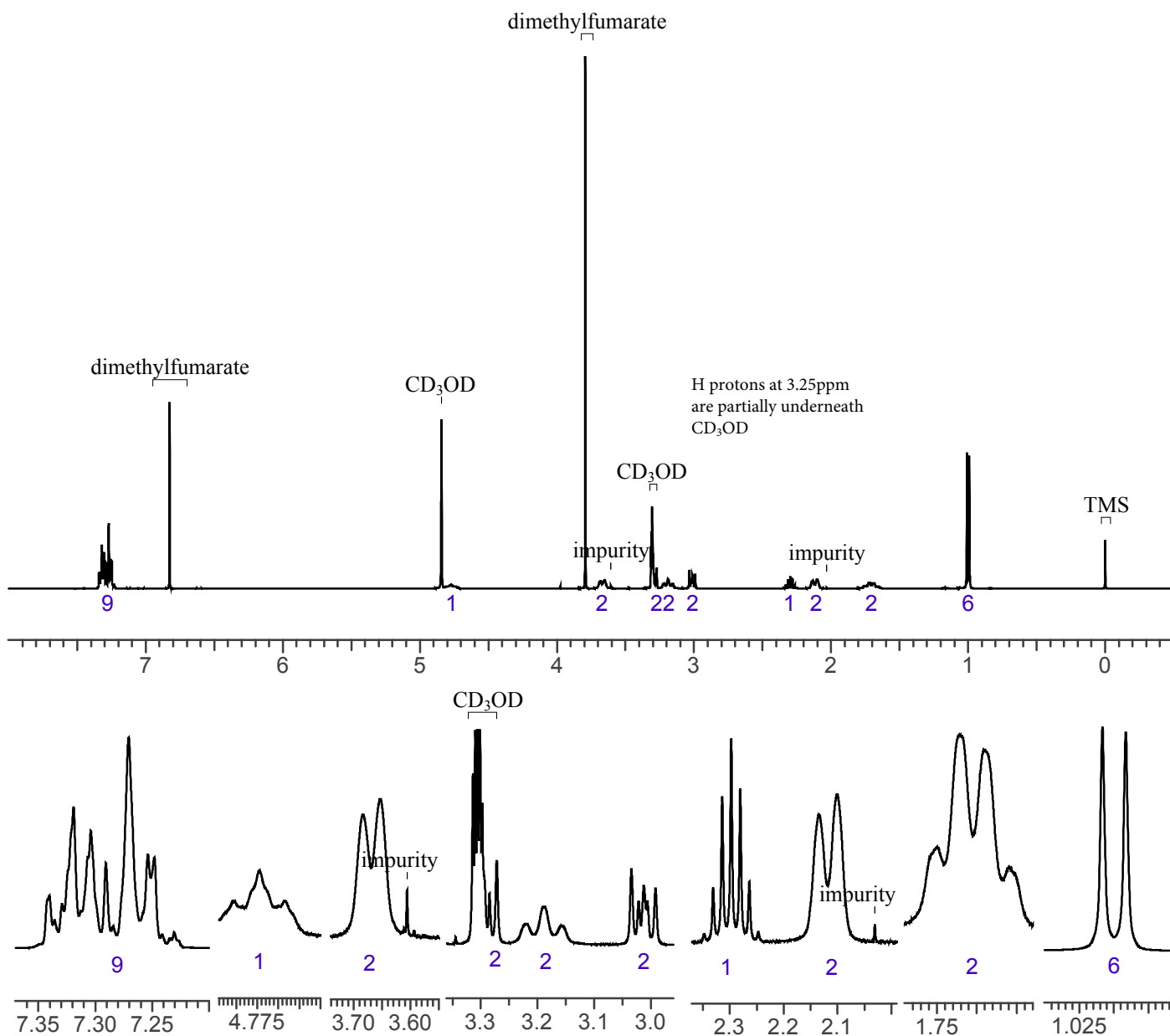
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in CD<sub>3</sub>OD 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

<sup>1</sup>H NMR: 4-Fluoroisobutyrylfentanyl HCl Lot# RM-160621-01; CD<sub>3</sub>OD; 400MHz





## 4-Fluoroisobutyrylfentanyl

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** HP-5; 30m x 0.25 mm x 0.25  $\mu$ m  
**Carrier Gas:** Helium at 1 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  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu

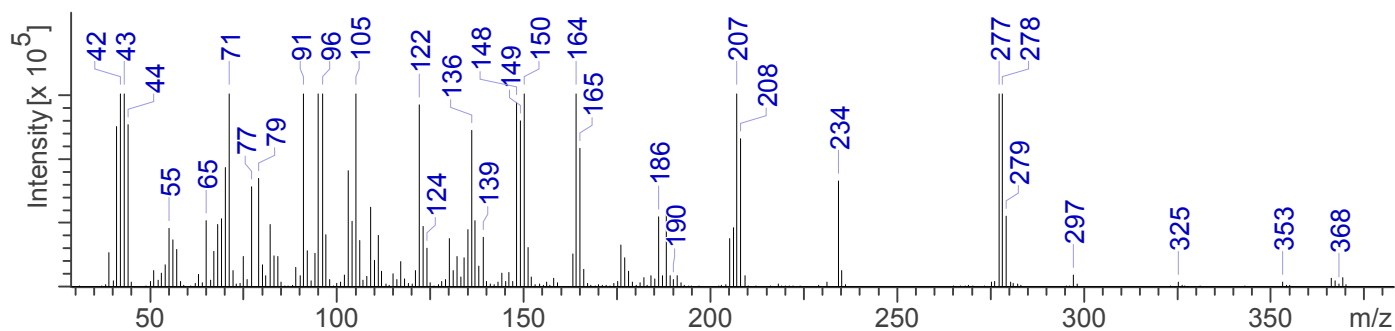
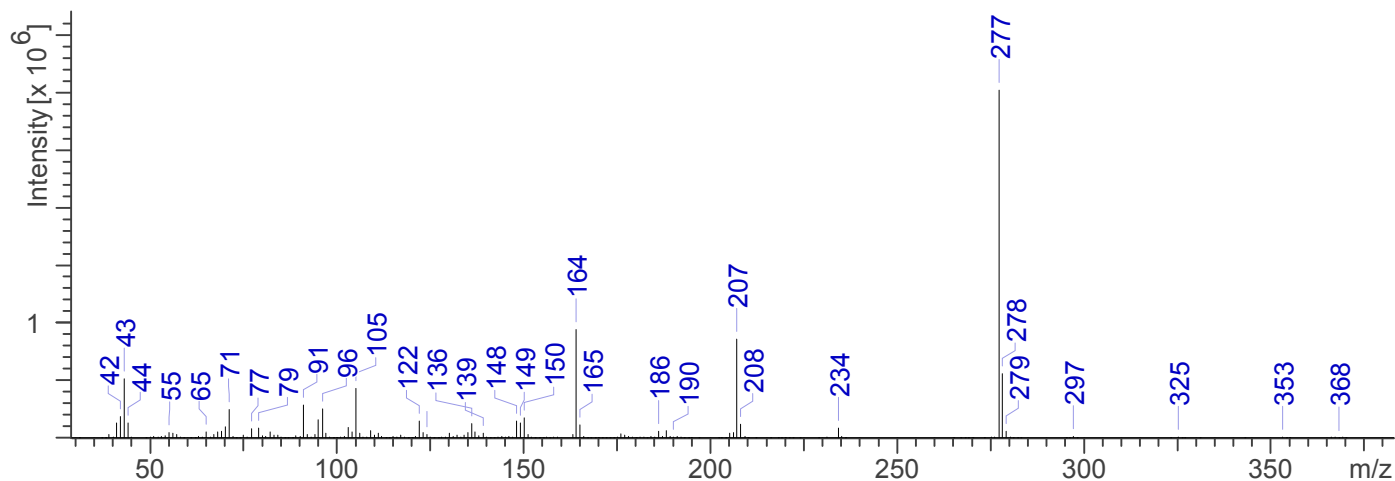
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 16.681 min

EI Mass Spectrum: 4-Fluoroisobutyrylfentanyl HCl; Lot# RM-160621-01





# 4-Fluoroisobutyrylfentanyl

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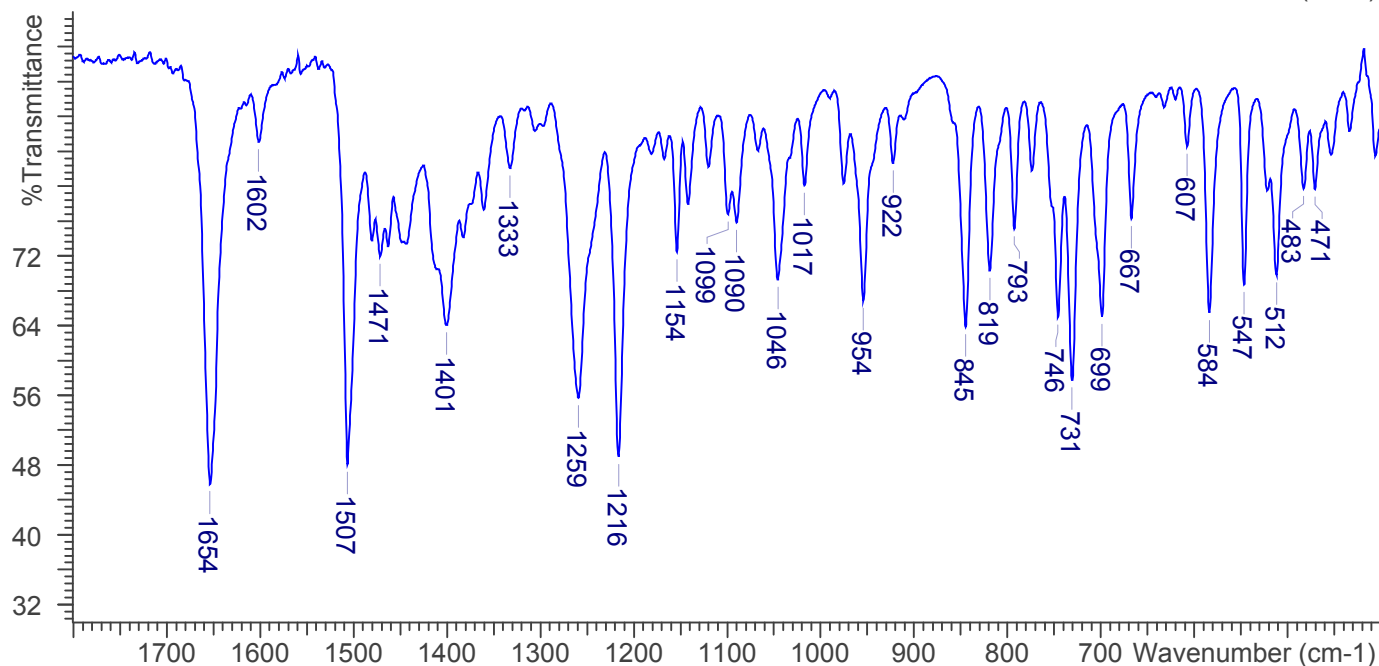
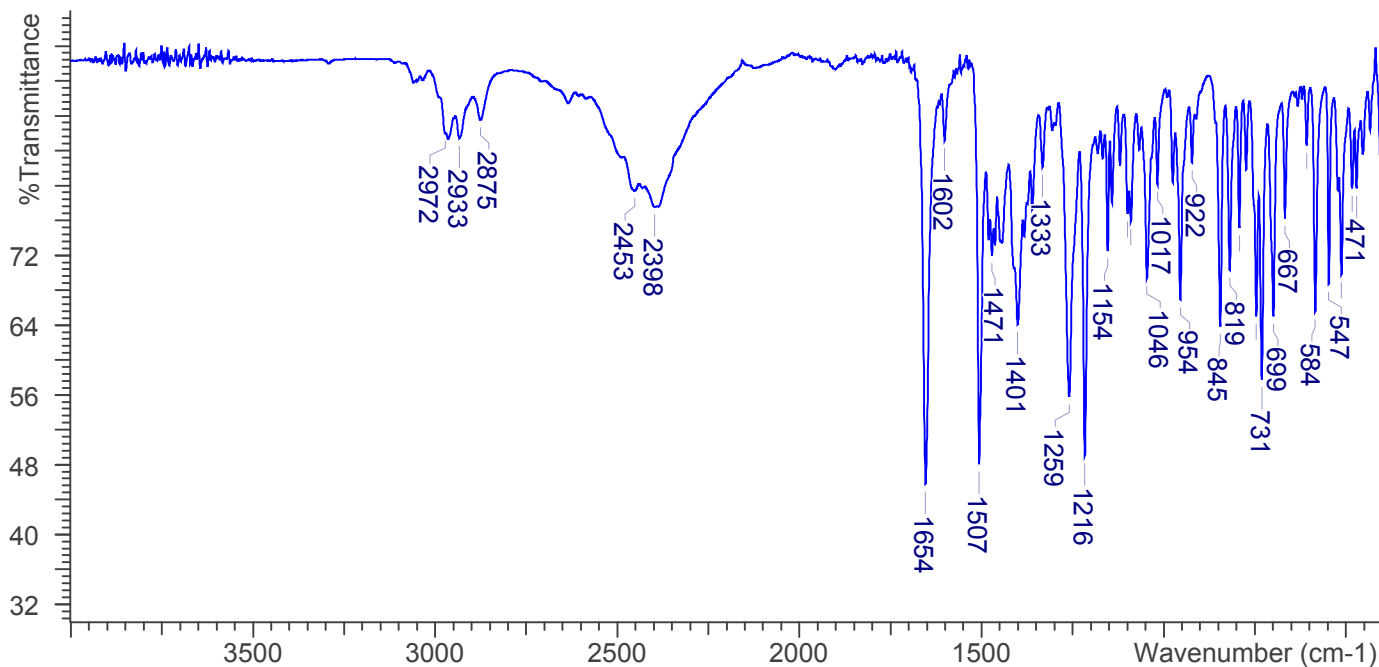


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 4-Fluoroisobutyrylfentanyl HCl Lot# RM-160621-01





## 4-Fluoroisobutyrylfentanyl

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### 4. ADDITIONAL RESOURCES

**No additional resources as of 11/15/16**