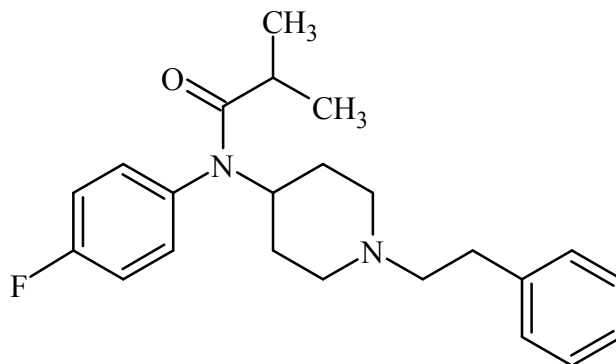




4-Fluoroisobutyrylfentanyl

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



1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -(4-fluorophenyl)- <i>N</i> -(1-phenethylpiperidin-4-yl)isobutyramide
CAS#:	NA
Synonyms:	<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
Source:	DEA Reference Material Collection
Appearance:	white powder (HCl)
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 FN ₂ O	368.48	NA
HCl	C ₂₃ H ₂₉ FN ₂ O · HCl	404.95	NA



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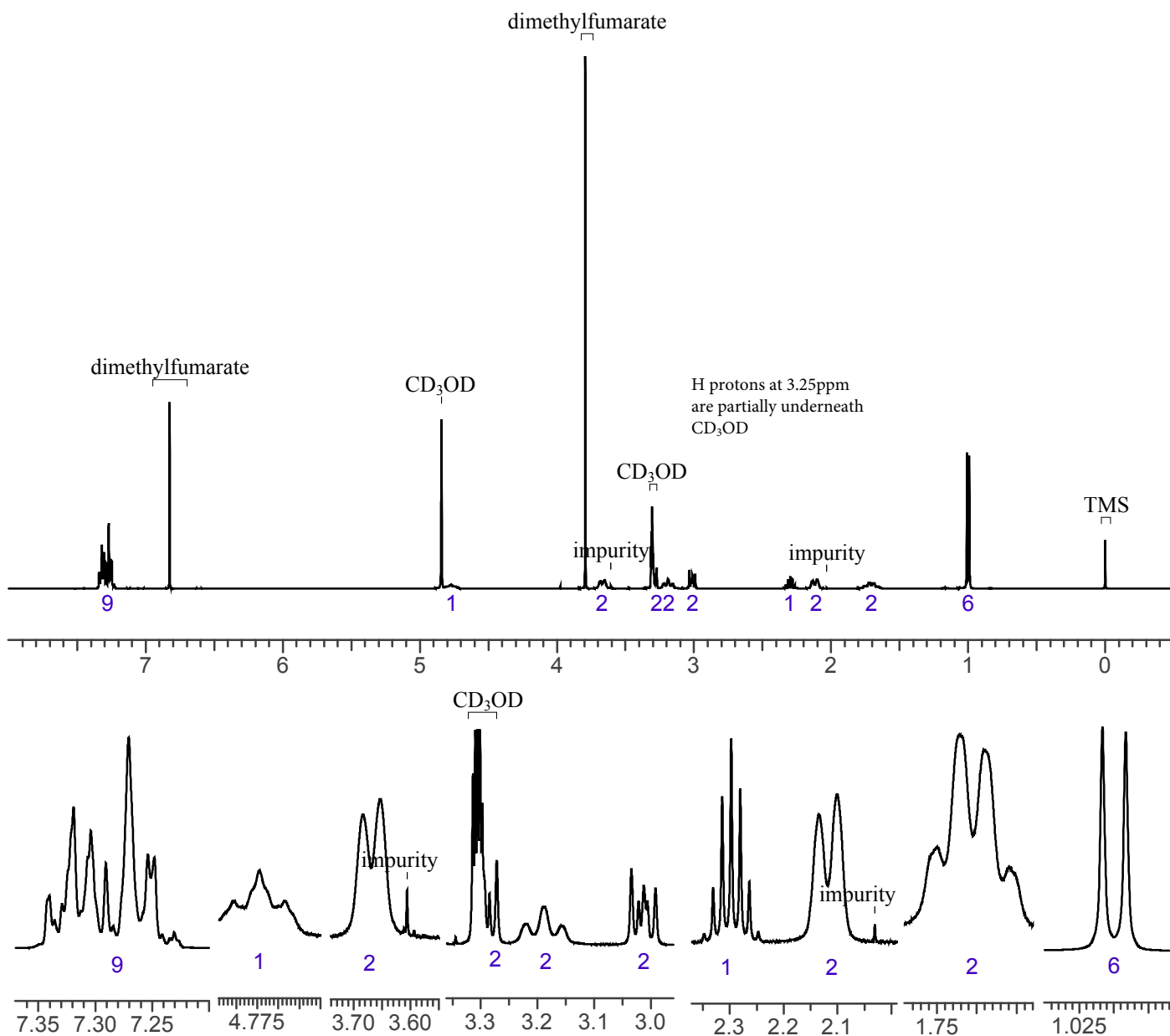
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/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

¹H NMR: 4-Fluoroisobutyrylfentanyl HCl Lot# RM-160621-01; CD₃OD; 400MHz





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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 μ 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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

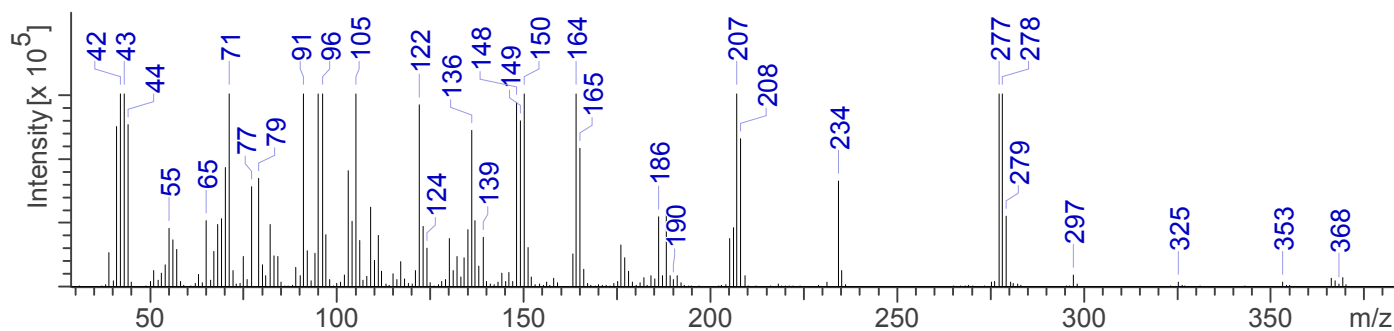
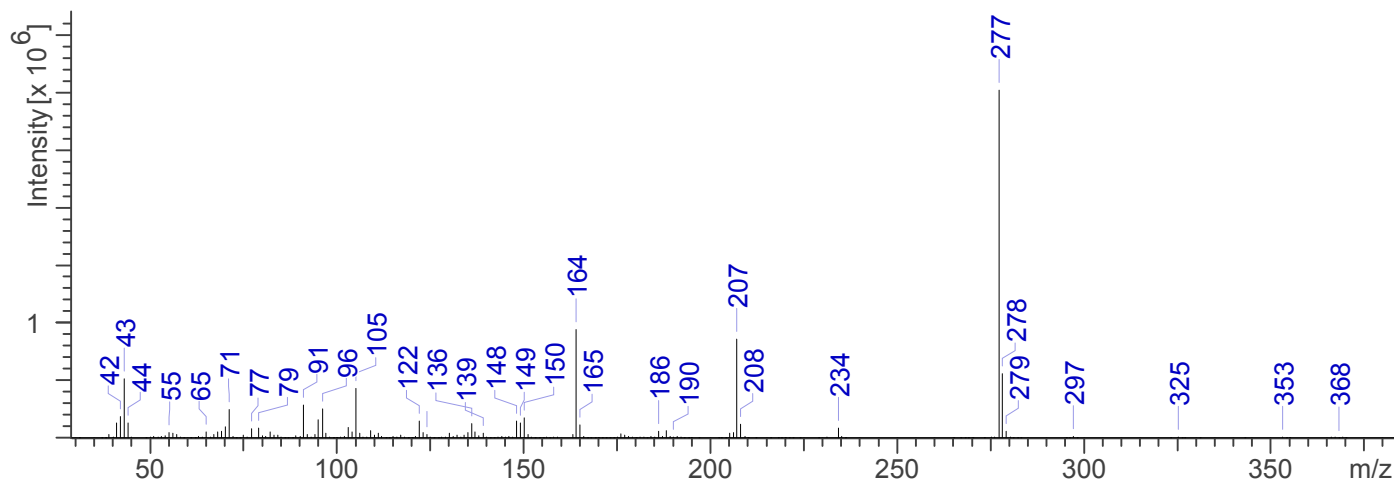
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.681 min

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





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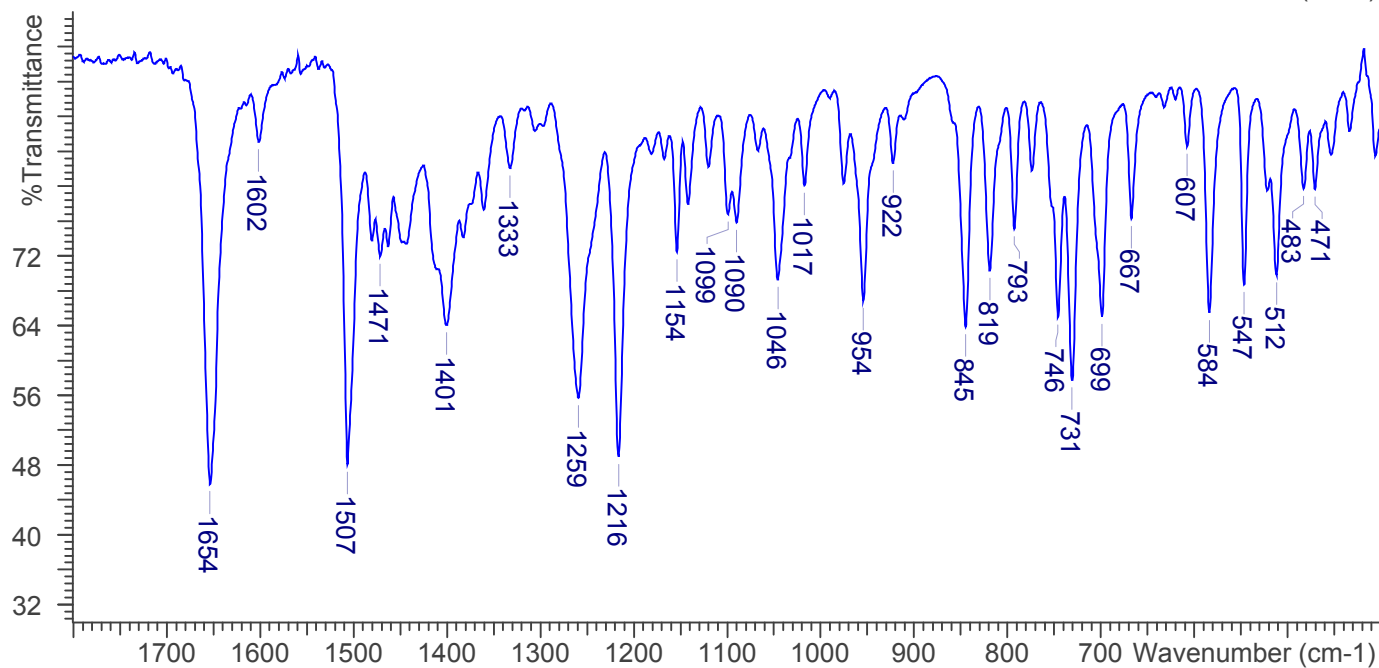
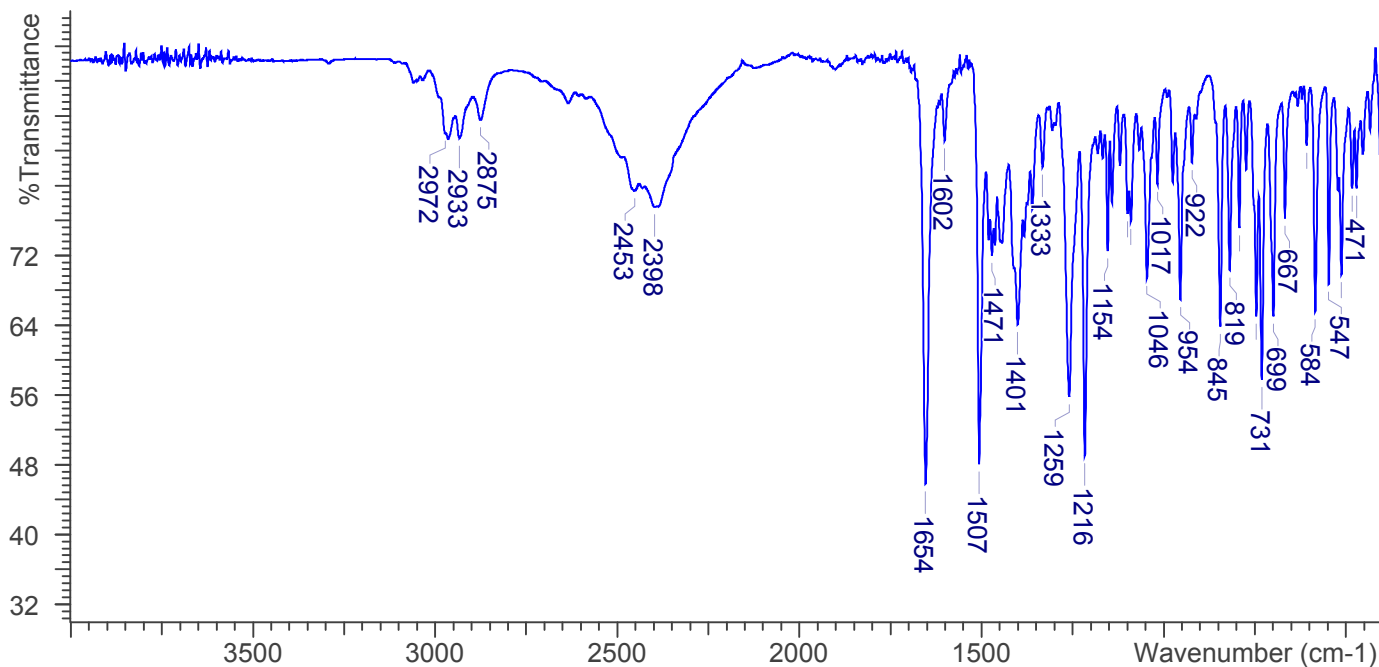


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
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