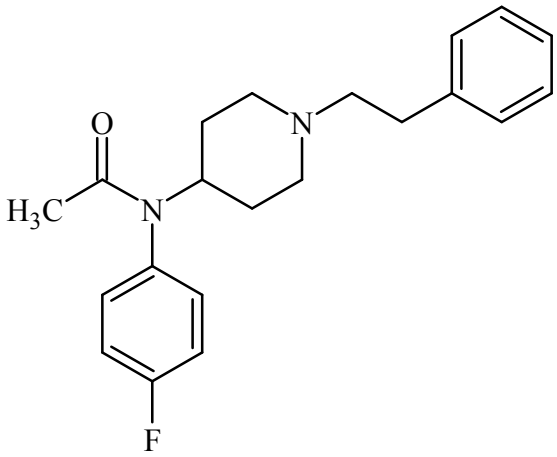
para-Fluoroacetyl fentanyl

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-phenethylpiperidin-4-yl)acetamide

CAS#: 104818-37-3

Synonyms: 4-fluoroacetyl fentanyl, p-fluoroacetyl fentanyl, NIH 10022, *N*-(4-fluorophenyl)-*N*-[1-(2-phenylethyl)piperidin-4-yl]acetamide

Source: DEA Reference Material Collection

Appearance: off-white powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{21}H_{25}FN_2O$	340.43	Not Determined
HCl	$C_{21}H_{25}FN_2O$ HCl	376.90	Not Determined

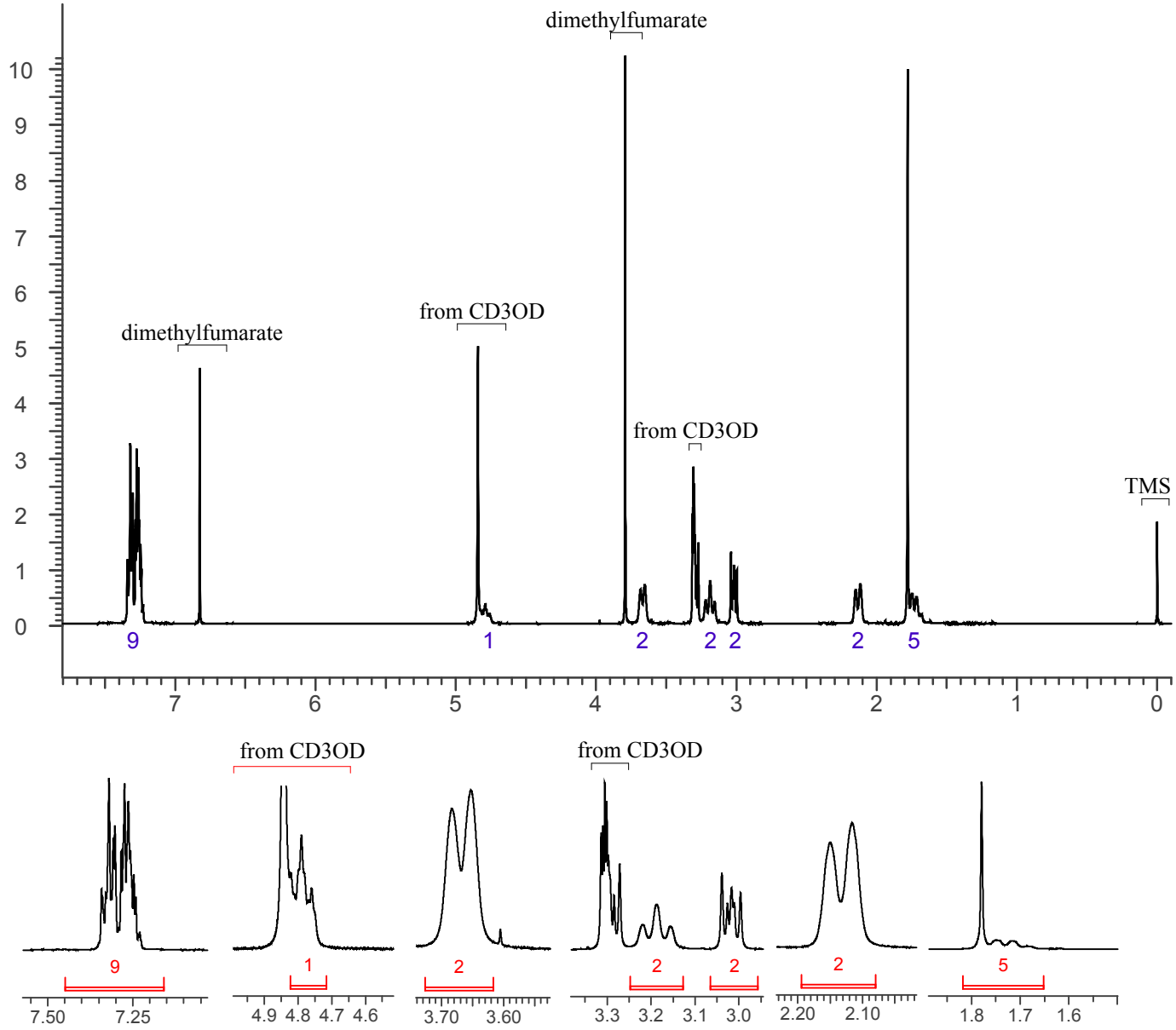
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~17 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 -3.0 ppm through 13.0 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}HNMR: para-Fluoroacetyl fentanyl HCl; Lot # 0539154-1; CD_3OD; 400MHz

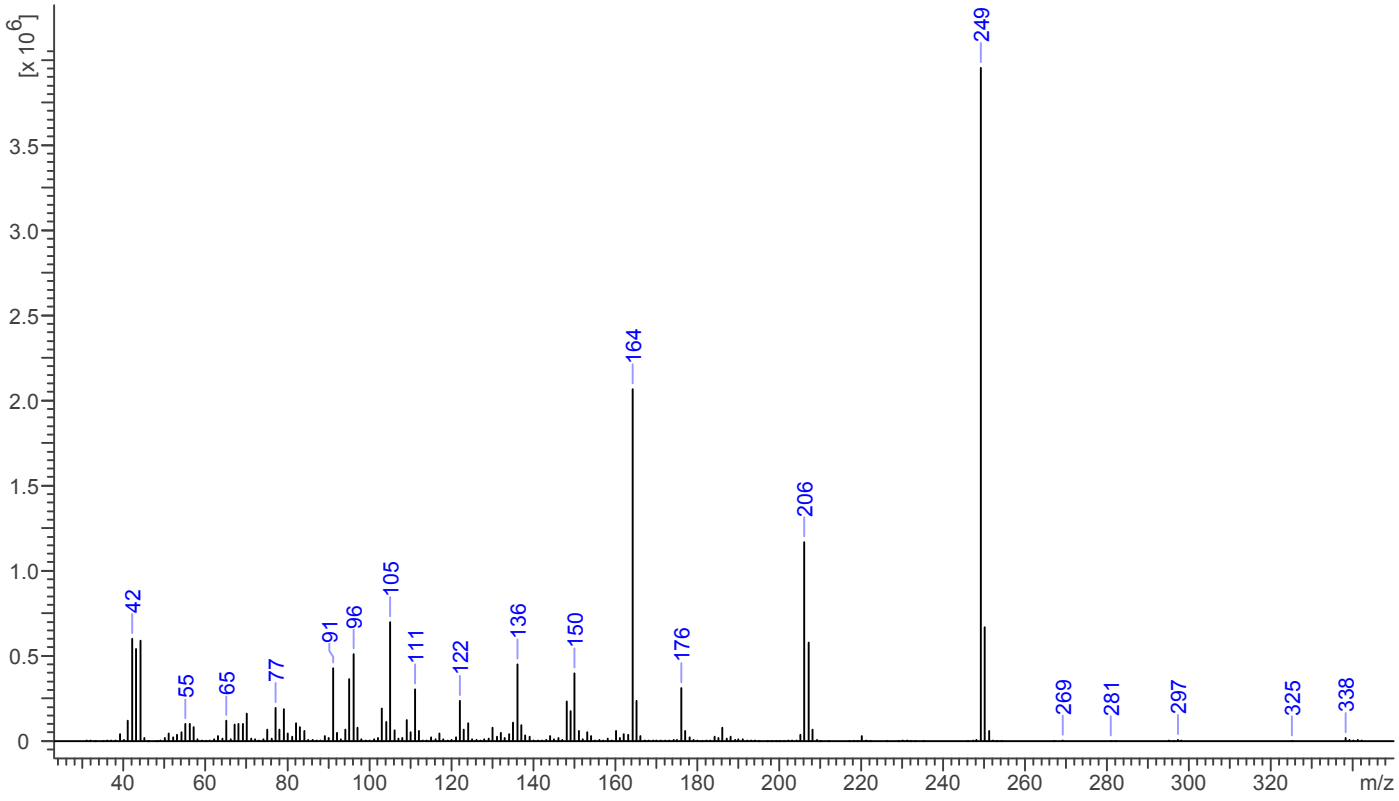


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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: 250
	Tune file: stune.u
	Acquisition mode: scan
Retention Time:	16.222 min

EI Mass Spectrum: para-Fluoroacetyl fentanyl HCl; Lot # 0539154-1



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-Fluoroacetyl fentanyl HCl; Lot # 0539154-1