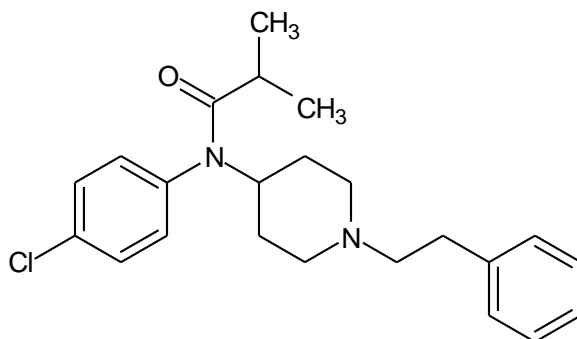




para-Chloro isobutyryl fentanyl

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-chlorophenyl)- <i>N</i> -(1-phenethylpiperidin-4-yl)isopropanamide
CAS#:	NA
Synonyms:	4-chloroisobutyryl fentanyl, 4-chloro iBF, <i>N</i> -(4-chlorophenyl)-2-methyl- <i>N</i> -[1-(2-phenylethyl)piperidin-4-yl]propanamide
Source:	DEA Reference Material Collection
Appearance:	White powder
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 ClN ₂ O	384.94	Not Determined
HCl	C ₂₃ H ₂₉ ClN ₂ O HCl	421.40	Not Determined



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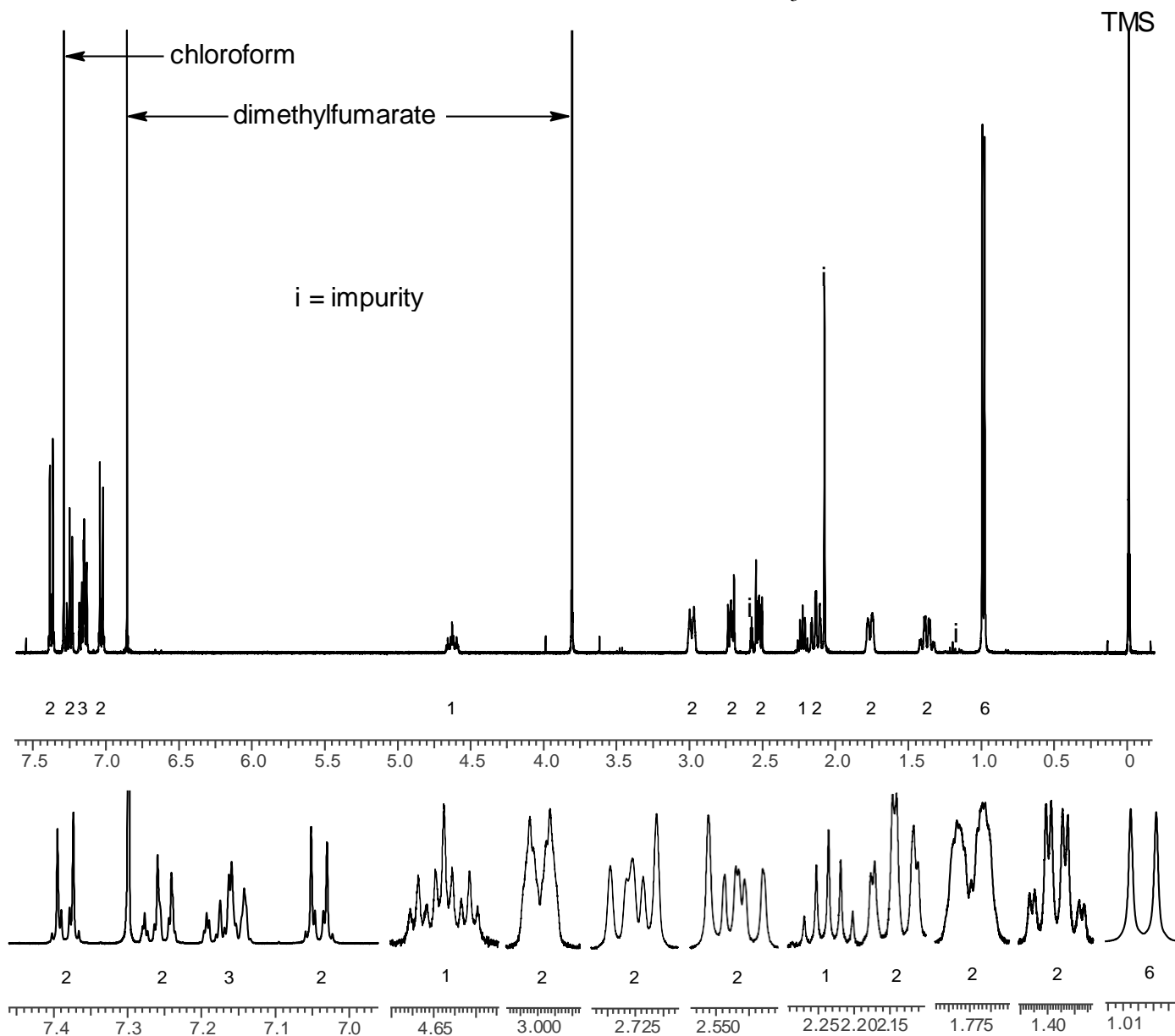
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Base extraction of analyte, diluted to ~13 mg/4mL in CDCl₃ 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: para-chloroisobutyryl fentanyl HCl; Lot# 0534601-1; CDCl₃; 400MHz; base extraction





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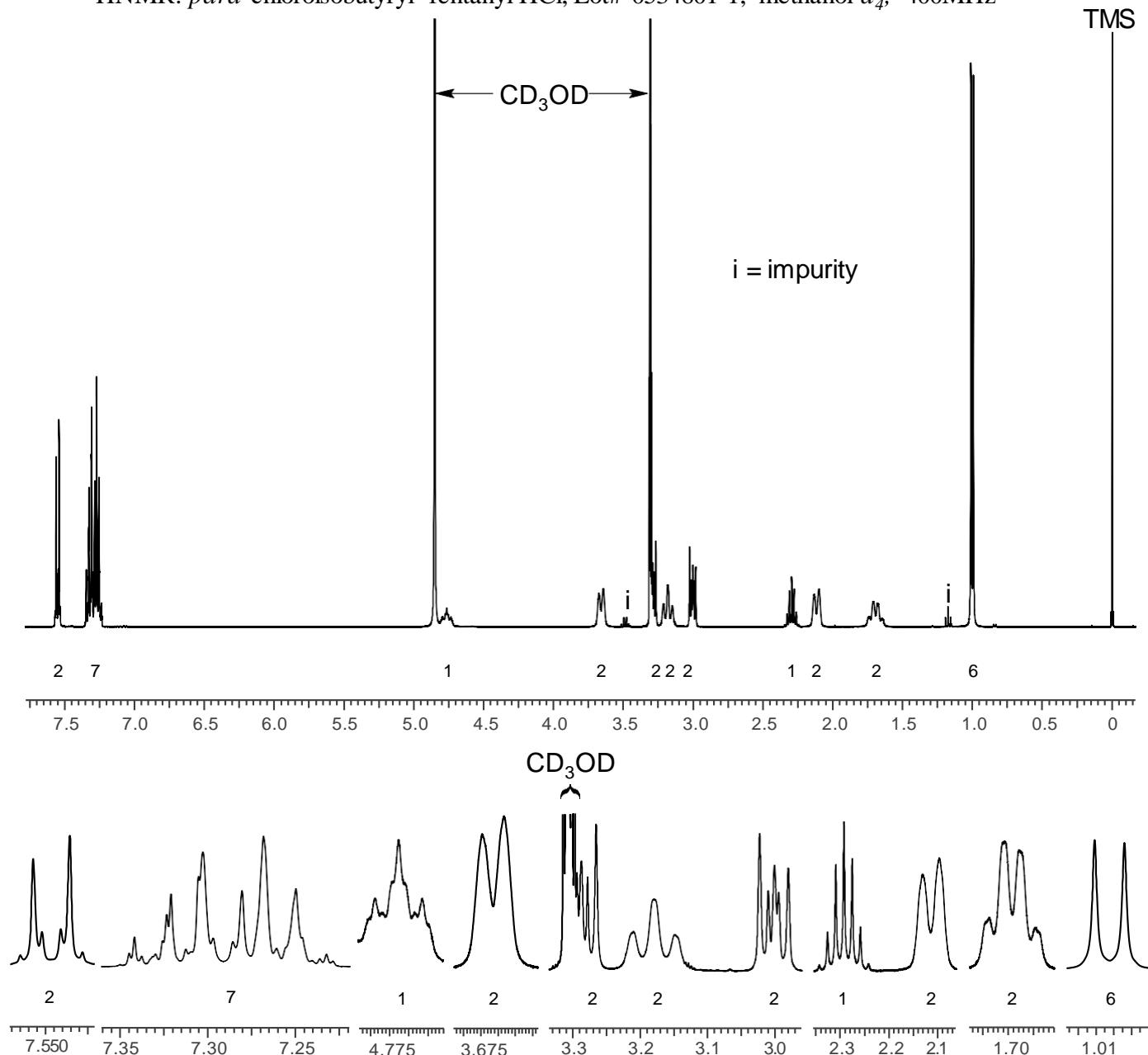


3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 mg/mL in methanol- d_4 containing TMS for 0 ppm reference.

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*-chloroisobutyryl fentanyl HCl; Lot# 0534601-1; methanol- d_4 ; 400MHz





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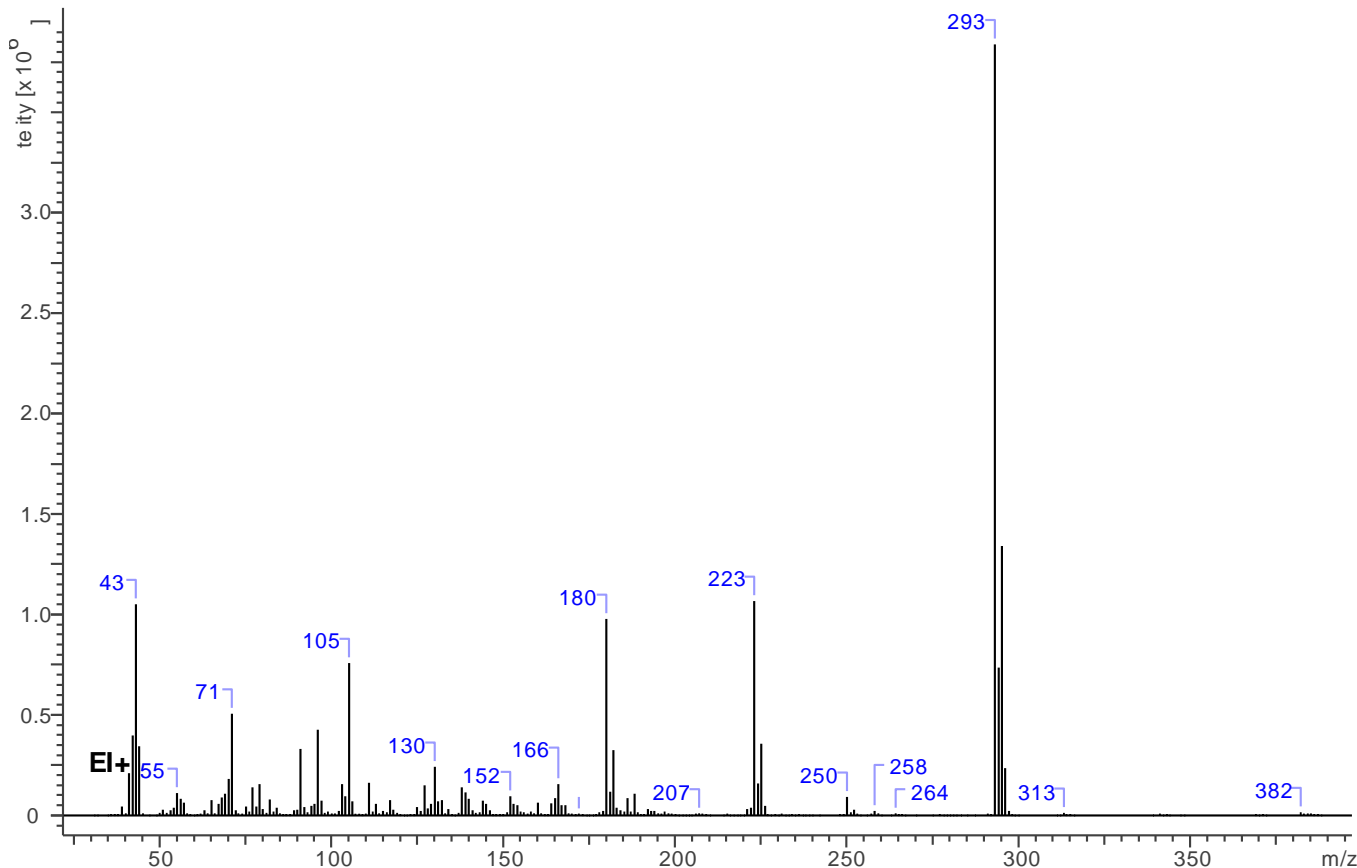
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

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 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: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 18.11 min

EI Mass Spectrum: *para*-chloroisobutyryl fentanyl HCl; Lot# 0534601-1





para-Chloro isobutyryl fentanyl

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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): *para*-chloroisobutyryl fentanyl HCl; Lot# 0534601-1

