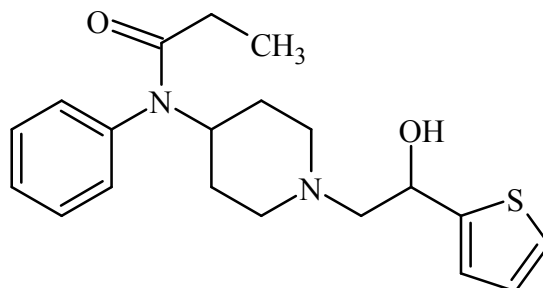




beta-Hydroxythiofentanyl

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



1. GENERAL INFORMATION

IUPAC Name: *N*-{1-[2-hydroxy-2-(thiophen-2-yl)ethyl]piperidin-4-yl}-*N*-phenylpropanamide

CAS#: NA

Synonyms: beta-Hydroxy-thiofentanyl

Source: DEA Reference Material Collection

Appearance: Off-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 ₂₀ H ₂₆ N ₂ O ₂ S	358.5	NA
HCl	C ₂₀ H ₂₆ N ₂ O ₂ S · HCl	394.9	NA



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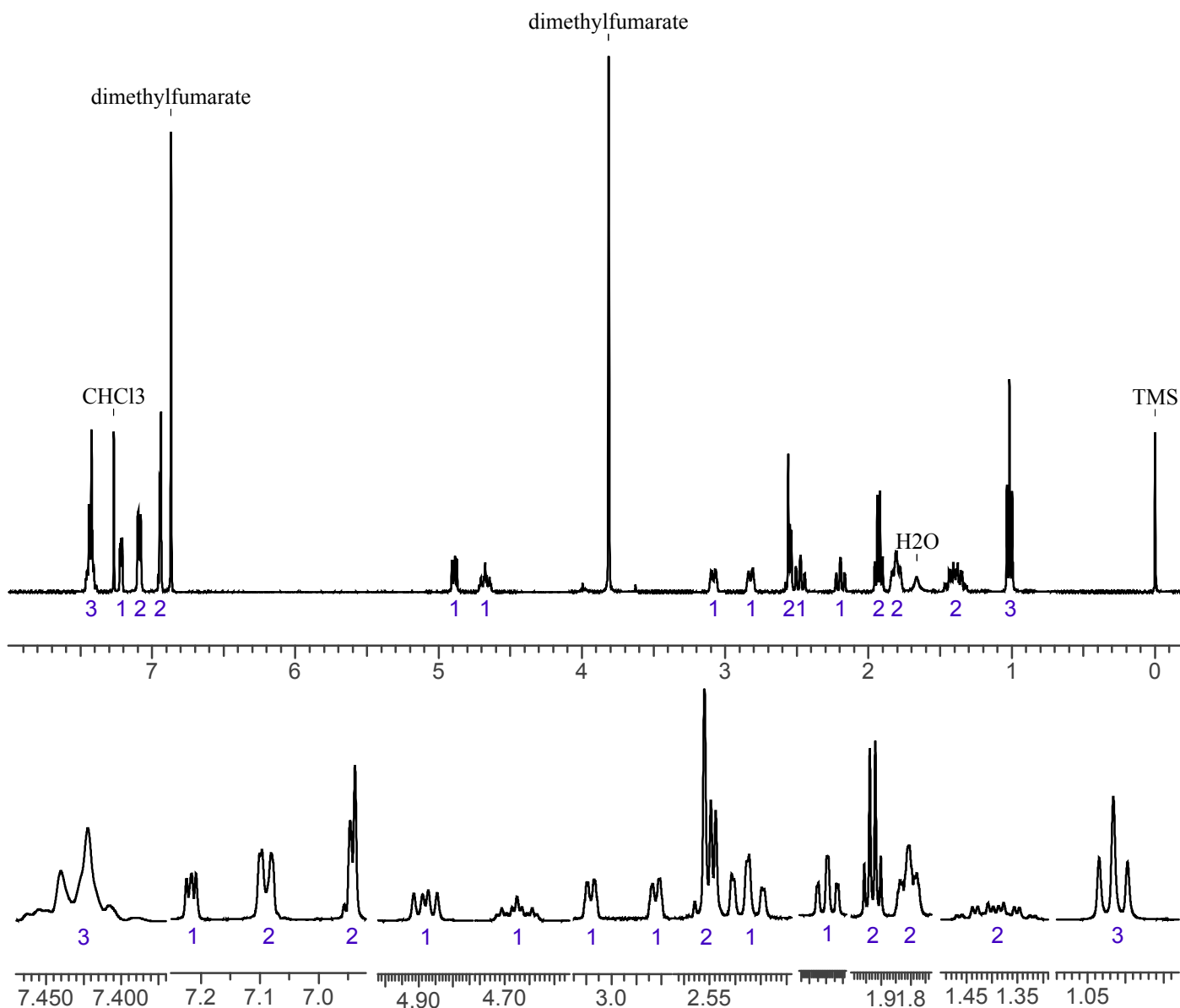
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~9 mg/mL base extracted 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

¹H NMR: *beta*-Hydroxythiofentanyl HCl Lot#RM-160417-01; CDCl₃; 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 (or equivalent); 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

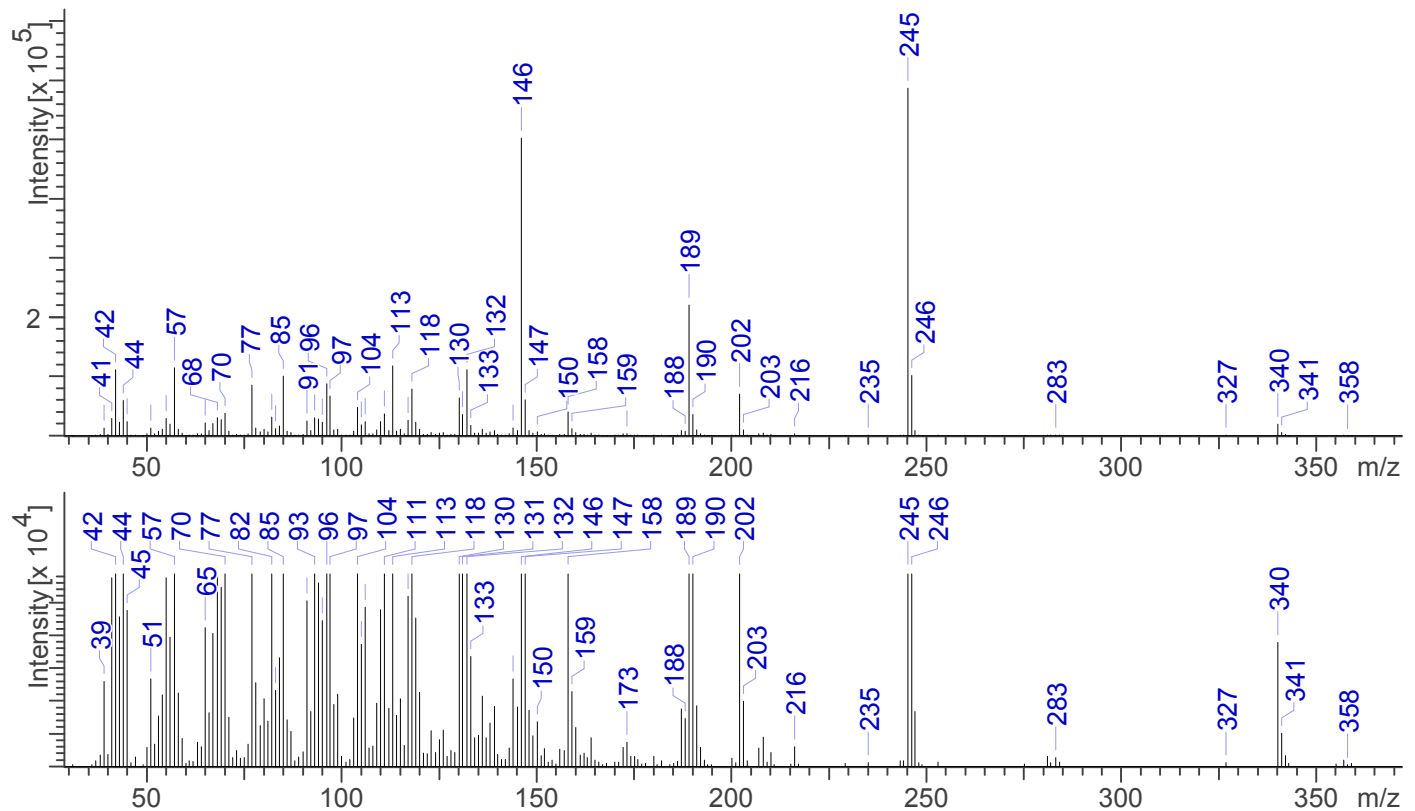
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 19.017 min

EI Mass Spectrum: *beta*-Hydroxythiofentanyl HCl lot# RM-160417-01





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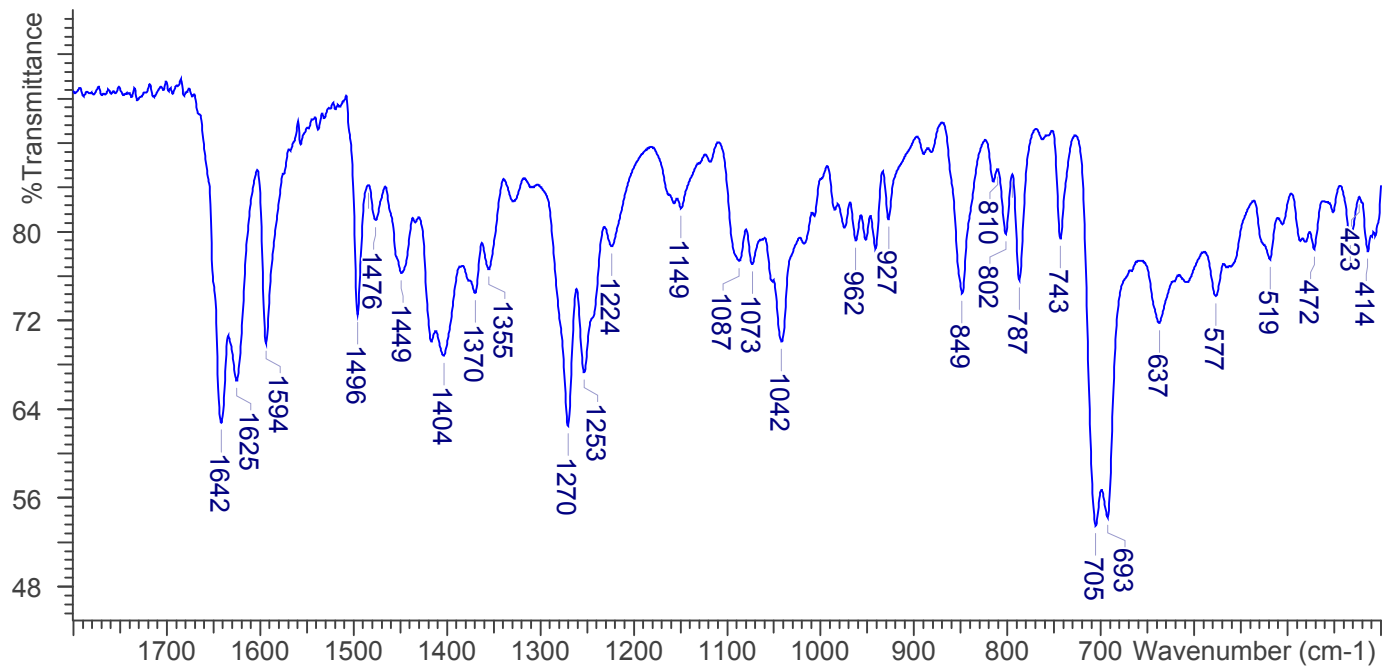
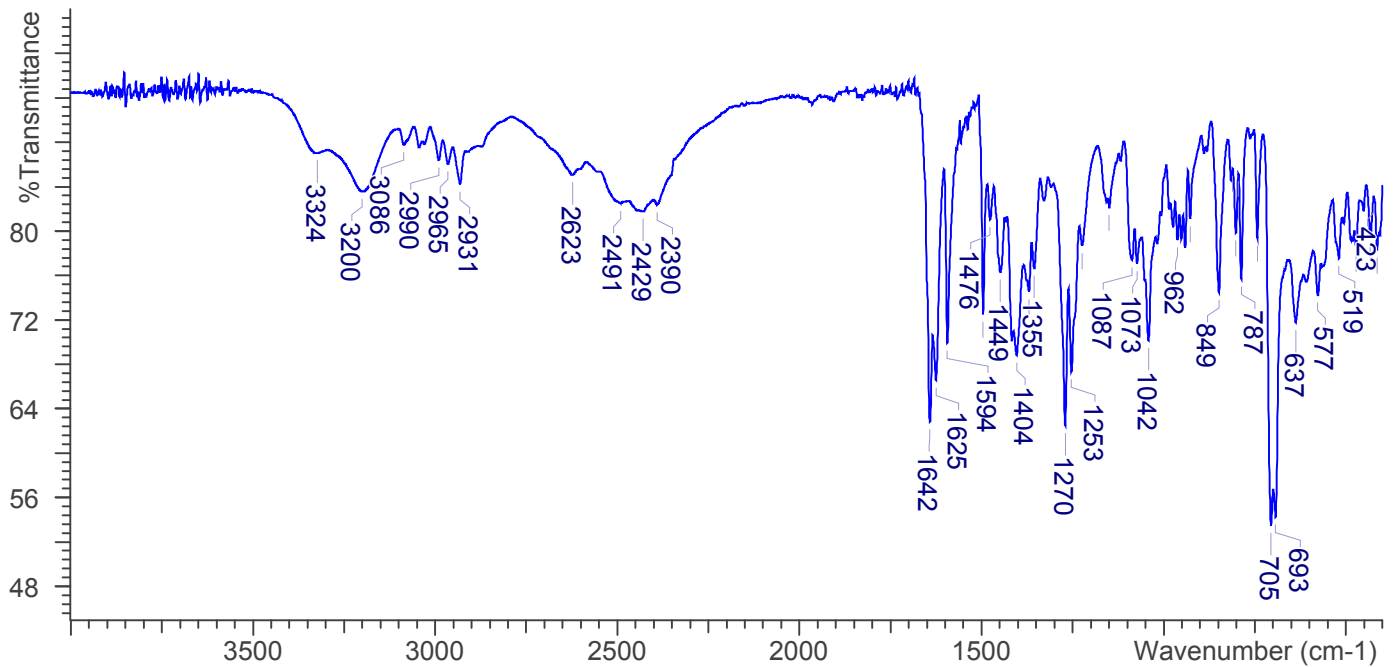


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 1
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): beta-Hydroxythiofentanyl HCl lot# RM-160417-01





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4. ADDITIONAL RESOURCES

No additional resources as of 02/28/17