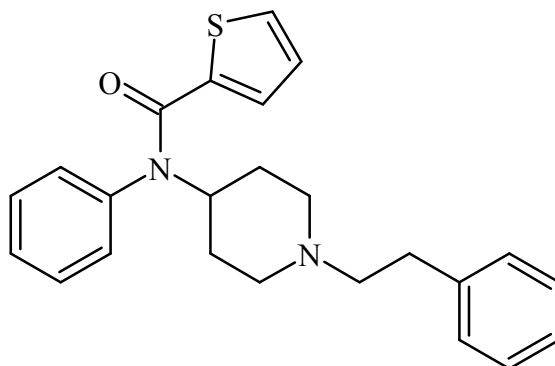




2-Thiophenoyl Fentanyl HCl

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



1. GENERAL INFORMATION

IUPAC Name: N-(2-phenethylpiperidin-4-yl)-N-phenylthiophene-2-carboxamide

CAS#: N/A

Synonyms: 2-Thiophene fentanyl, 2-Thiofuranyl fentanyl,
N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]thiophene-2-carboxamide

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 ₂₄ H ₂₆ N ₂ OS	390.54	Not Determined
HCl	C ₂₄ H ₂₆ N ₂ OS HCl	427.00	Not Determined



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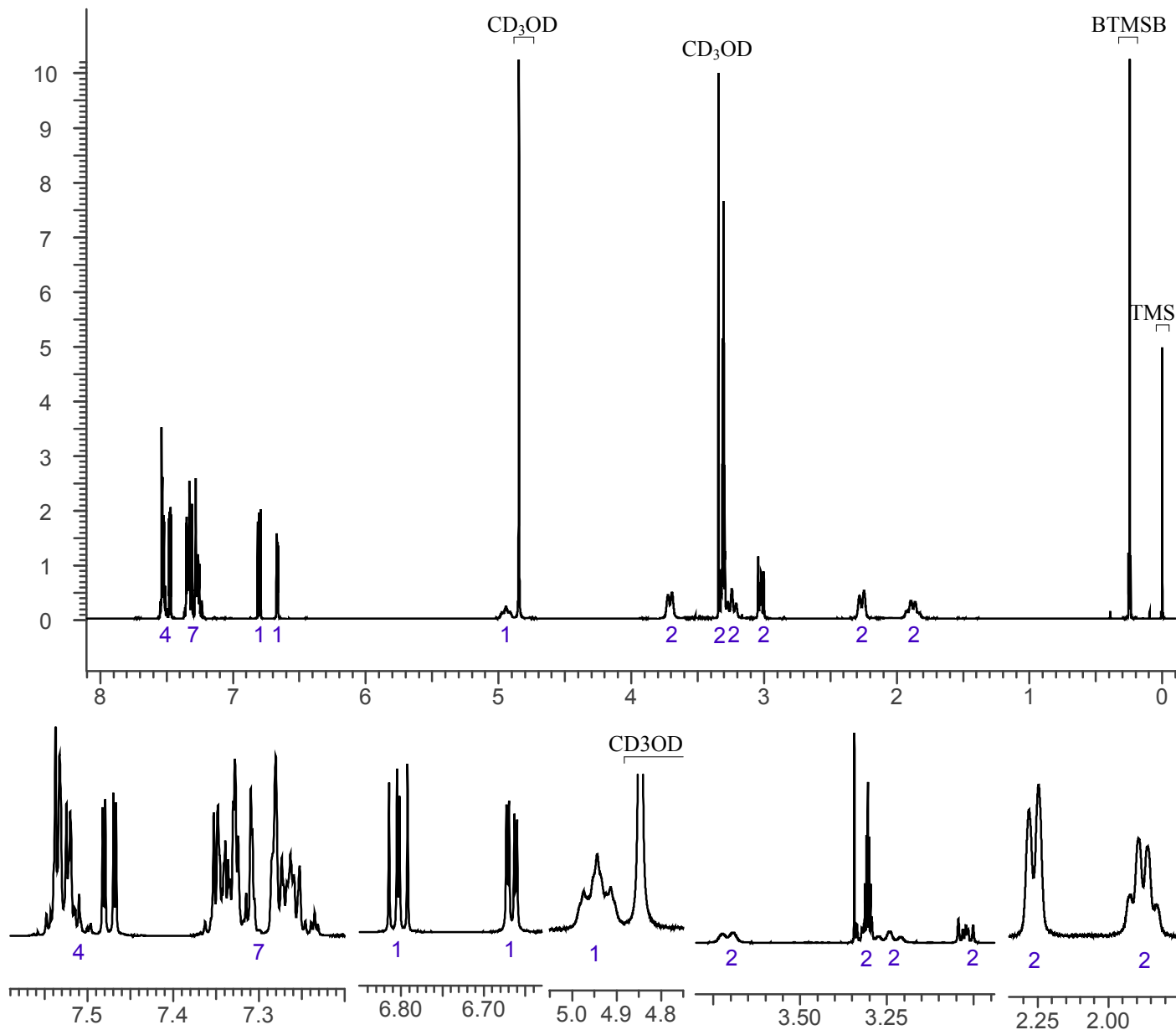
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in CD₃OD containing TMS for 0 ppm reference and 1,4-BTMSB-d₄ 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

¹HNMR: 2-Thiophenoyl Fentanyl HCl, Lot RM-170825-01, CD₃OD; 400MHz





2-Thiophenoyl Fentanyl HCl

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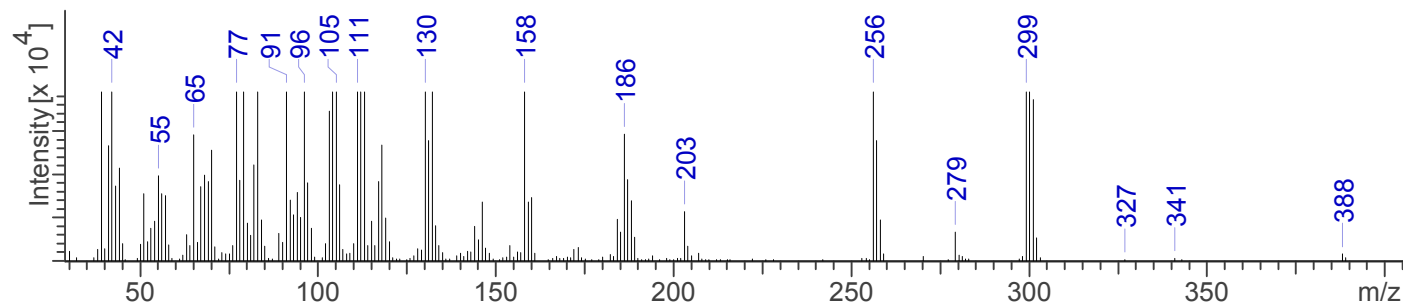
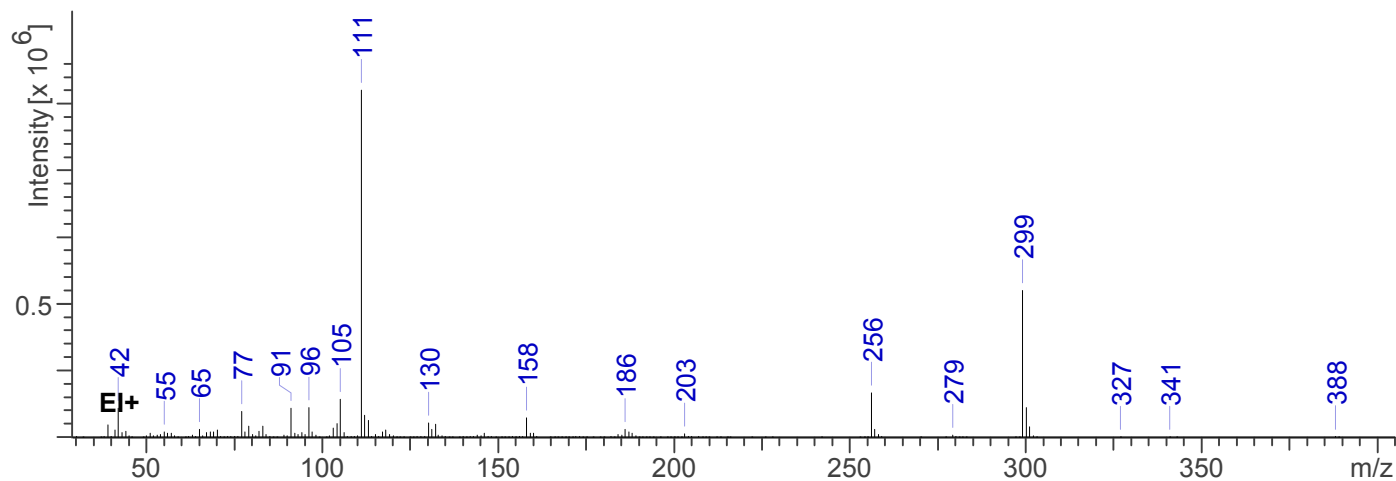
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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 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: 250
Tune file: stune.u
Acquisition mode: scan
Retention Time: 23.993 min

EI Mass Spectrum: 2-Thiophenoyl fentanyl HCl, Lot RM-170825-01





2-Thiophenoyl Fentanyl HCl

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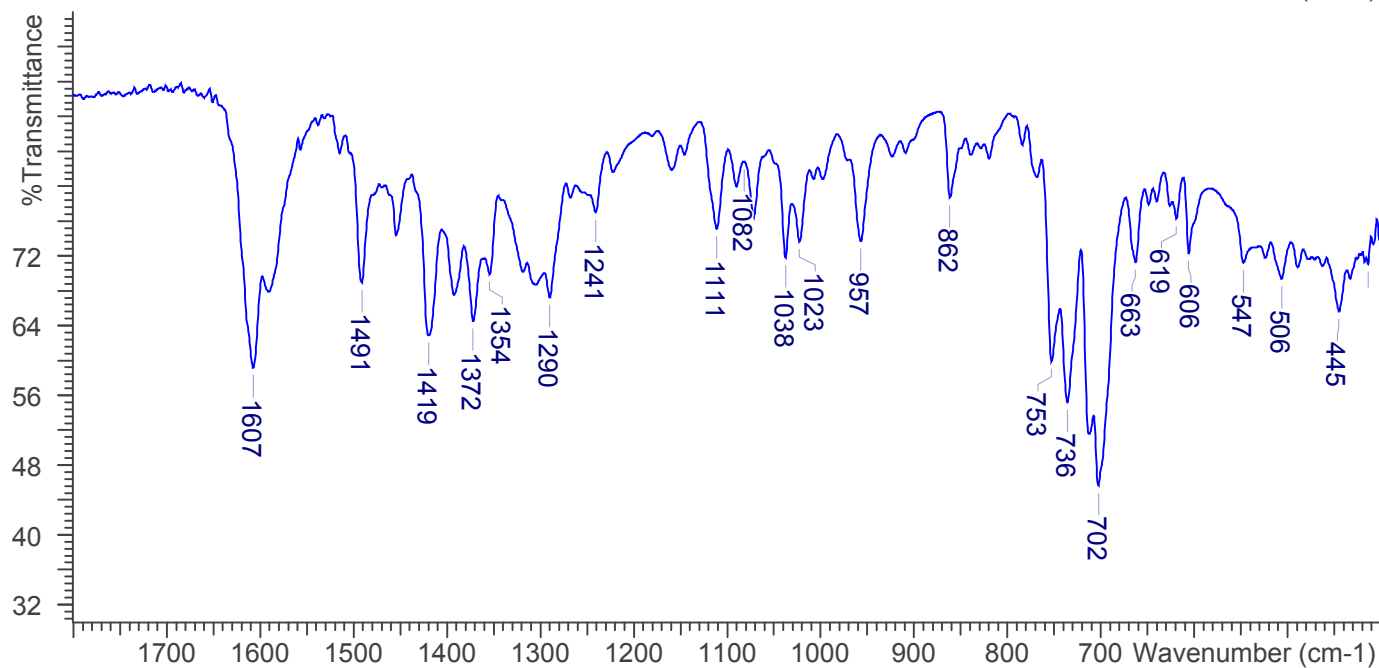
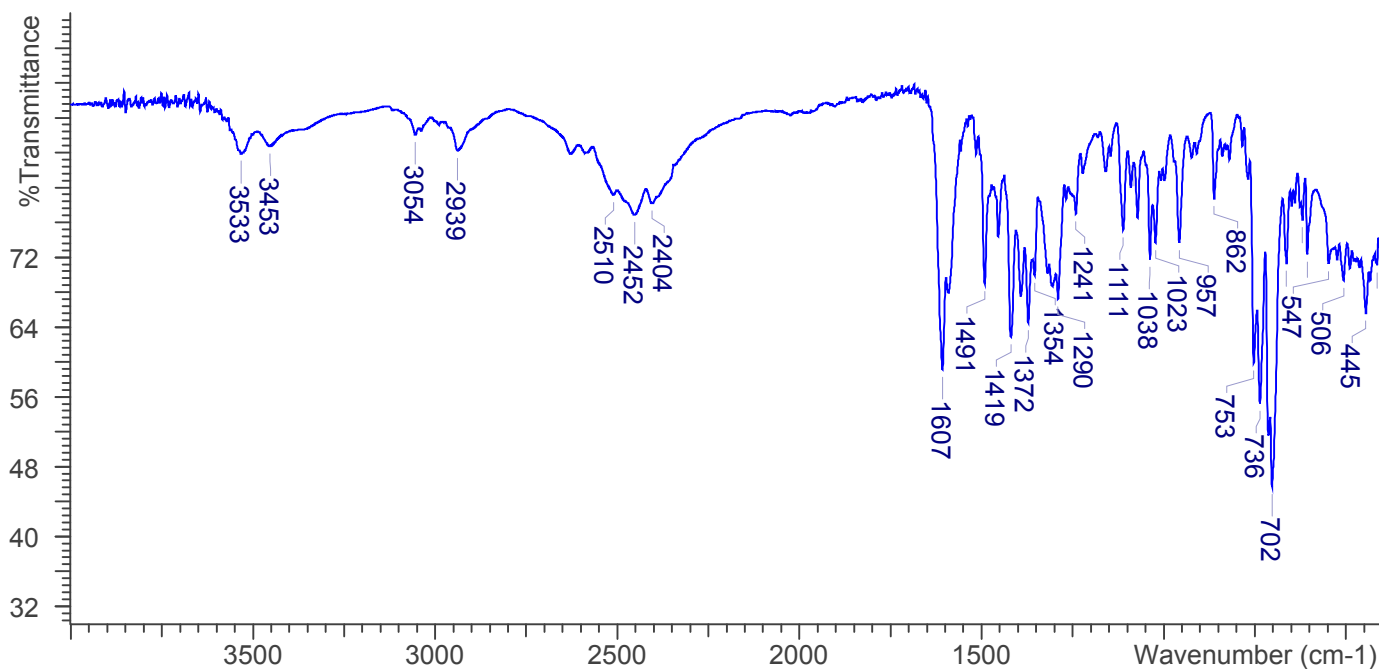


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 2-Thiophenoyl Fentanyl HCl; Lot RM-170825-01





2-Thiophenoyl Fentanyl HCl

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4. ADDITIONAL RESOURCES

No Literature available as of 11/2017