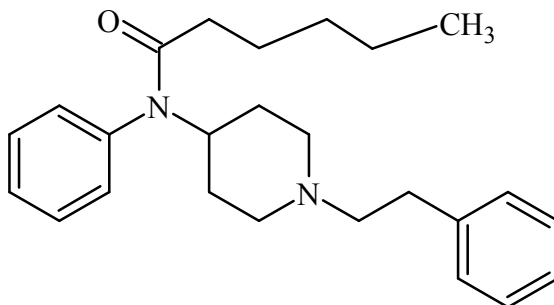




Hexanoyl fentanyl

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> -phenyl- <i>N</i> -[1-(2-phenylethyl)piperidin-4-yl]hexanamide
CAS#:	NA
Synonyms:	<i>N</i> -(1-Phenethylpiperidin-4-yl) <i>N</i> -phenylhexanamide, Hexanoylfentanyl
Source:	DEA Reference Material Collection
Appearance:	white powder
UV_{max}(nm):	NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₅ H ₃₄ N ₂ O	378.55	Not Determined
HCl	C ₂₅ H ₃₄ N ₂ O · HCl	415.01	Not Determined



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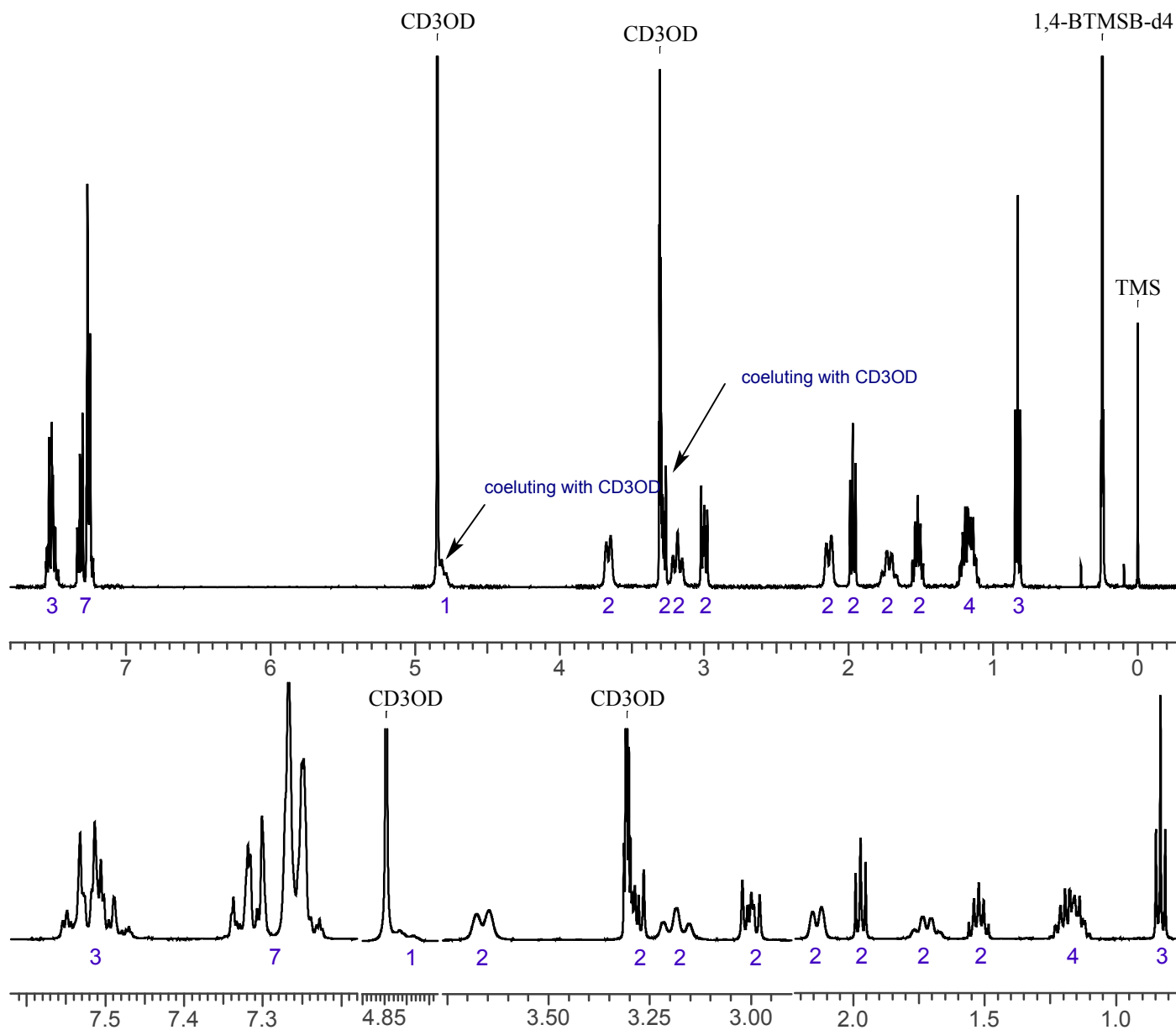


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 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 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
¹HNMR: Hexanoyl fentanyl HCl Lot# ALB-297-7; CD₃OD; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

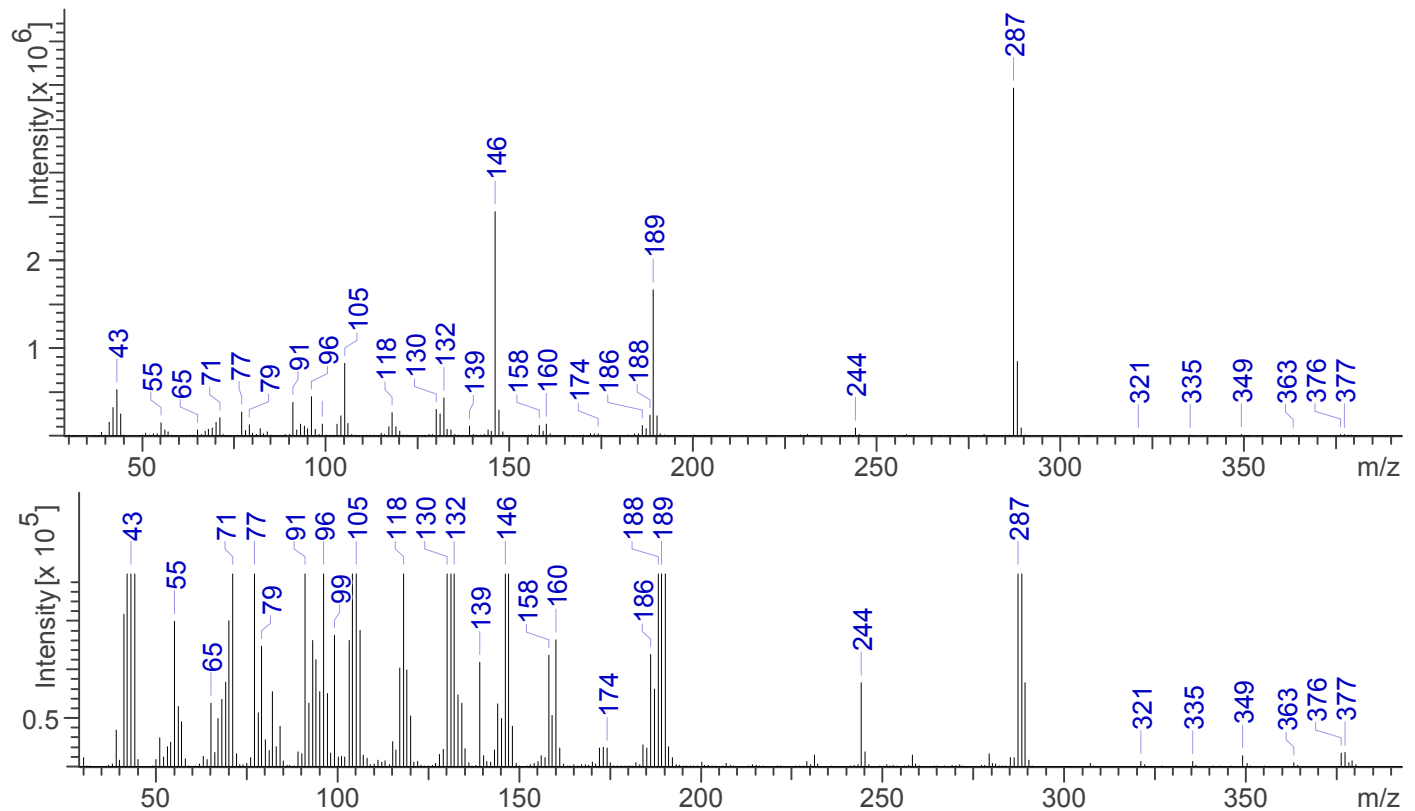
Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

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 1.5 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: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 19.544 min

EI Mass Spectrum: Hexanoyl fentanyl HCl Lot# ALB-297-7





Hexanoyl fentanyl



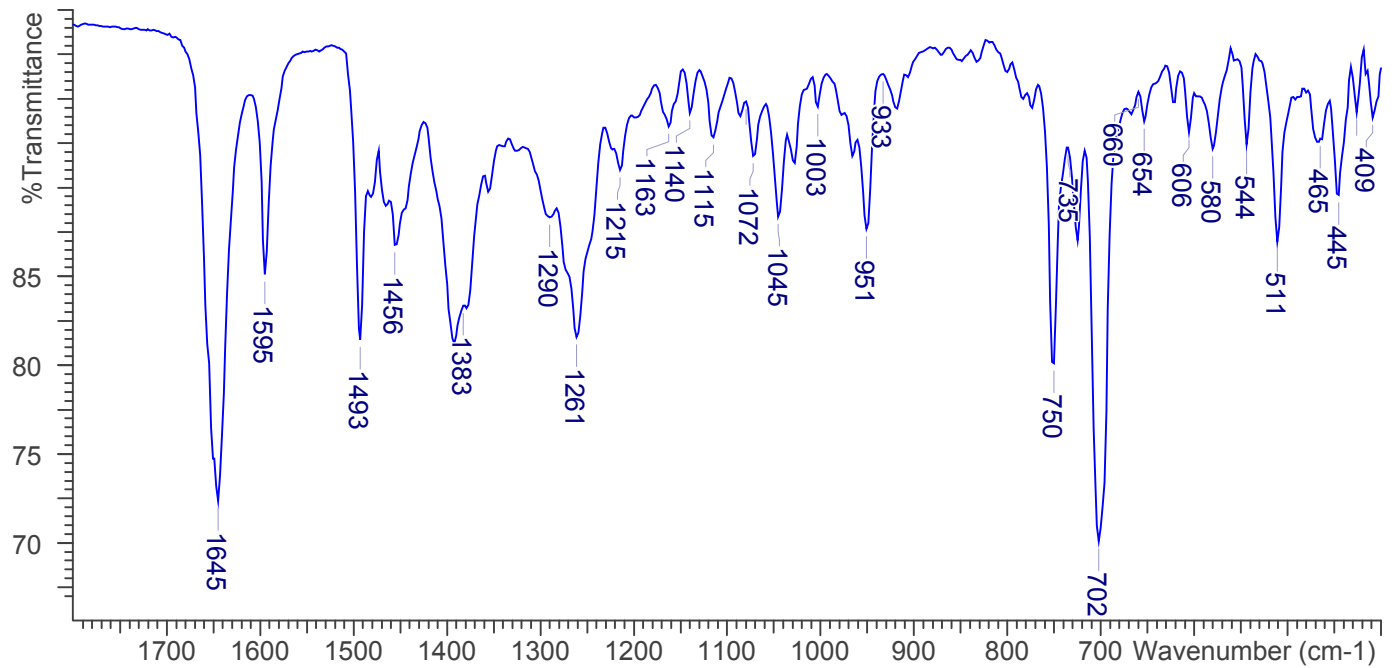
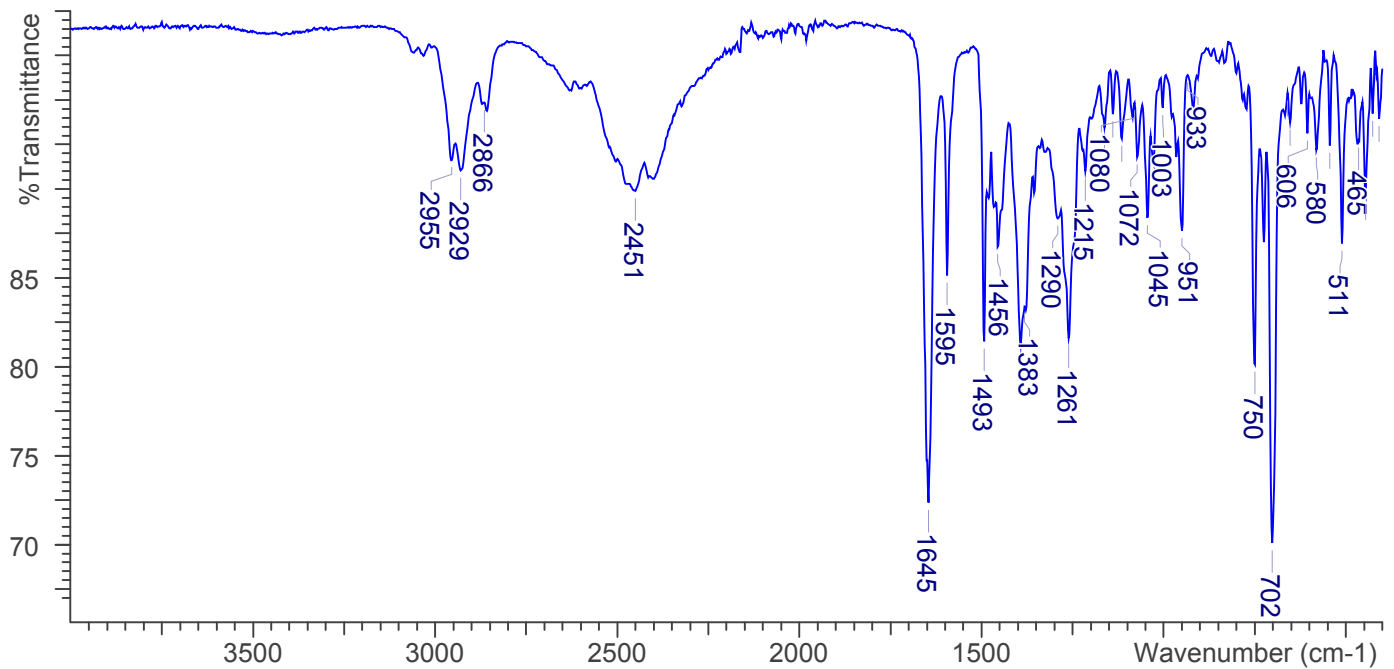
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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR (Smart Golden Gate ATR Accessory)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR (Smart Golden Gate ATR Accessory): Hexanoyl fentanyl HCl Lot# ALB-297-7





Hexanoyl fentanyl

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4. ADDITIONAL RESOURCES

No additional resources as of 08/24/17