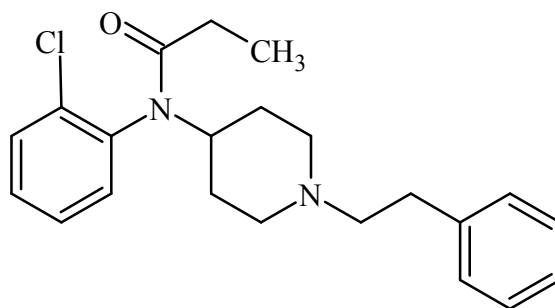




ortho-Chlorofentanyl

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-chlorophenyl)-N-(1-phenethylpiperidin-4-yl)propionamide

CAS#: N/A

Synonyms: N-(2-chlorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide, o-Chlorofentanyl

Source: DEA Reference Material Collection

Appearance: white powder

UV_{max}(nm): N/A

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₂ H ₂₇ ClN ₂ O	370.92	NA
HCl	C ₂₂ H ₂₇ ClN ₂ O · HCl	407.38	NA



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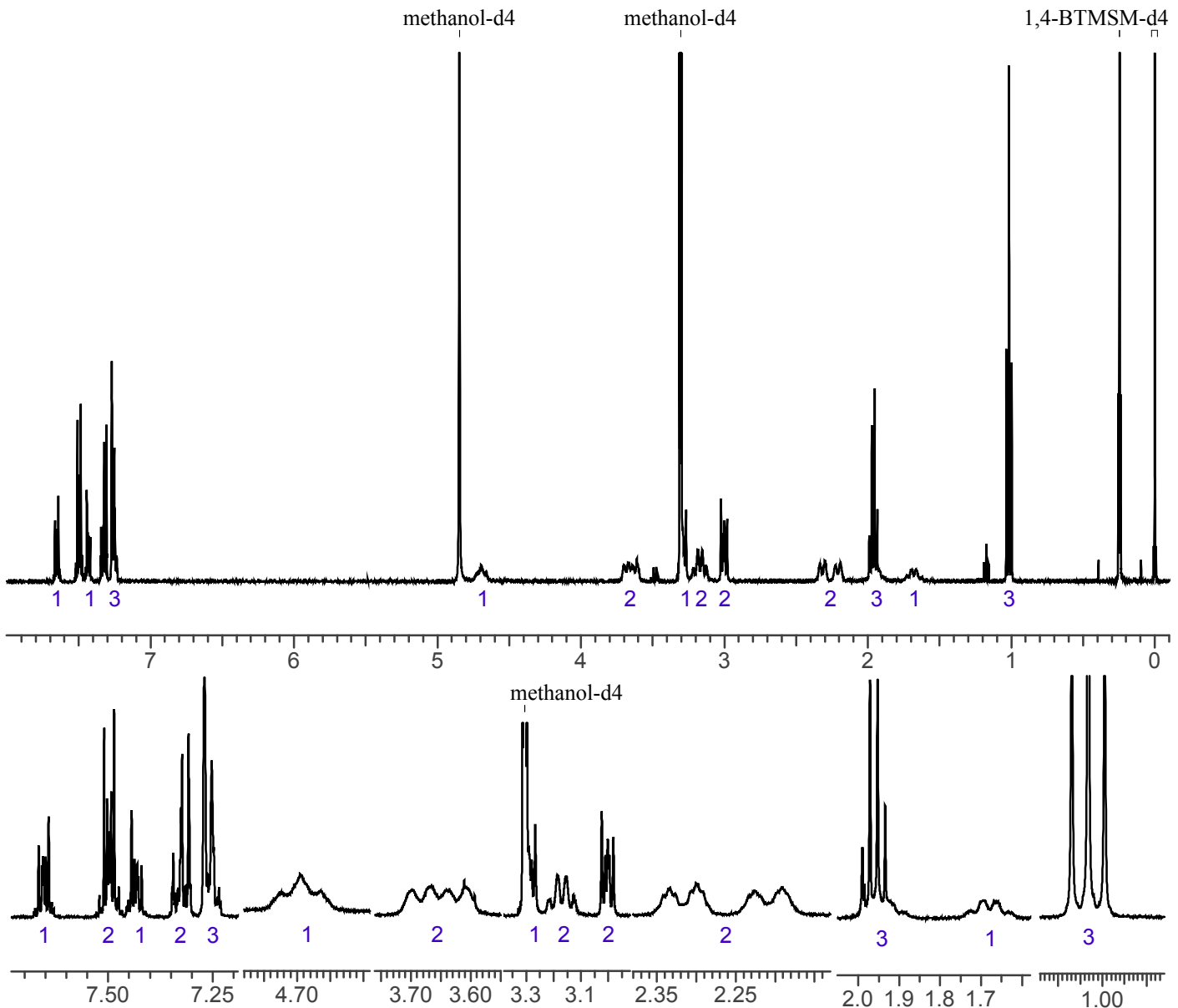
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~4 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: ortho-Chlorofentanyl HCl; Lot# 0600281-13; CD₃OD; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

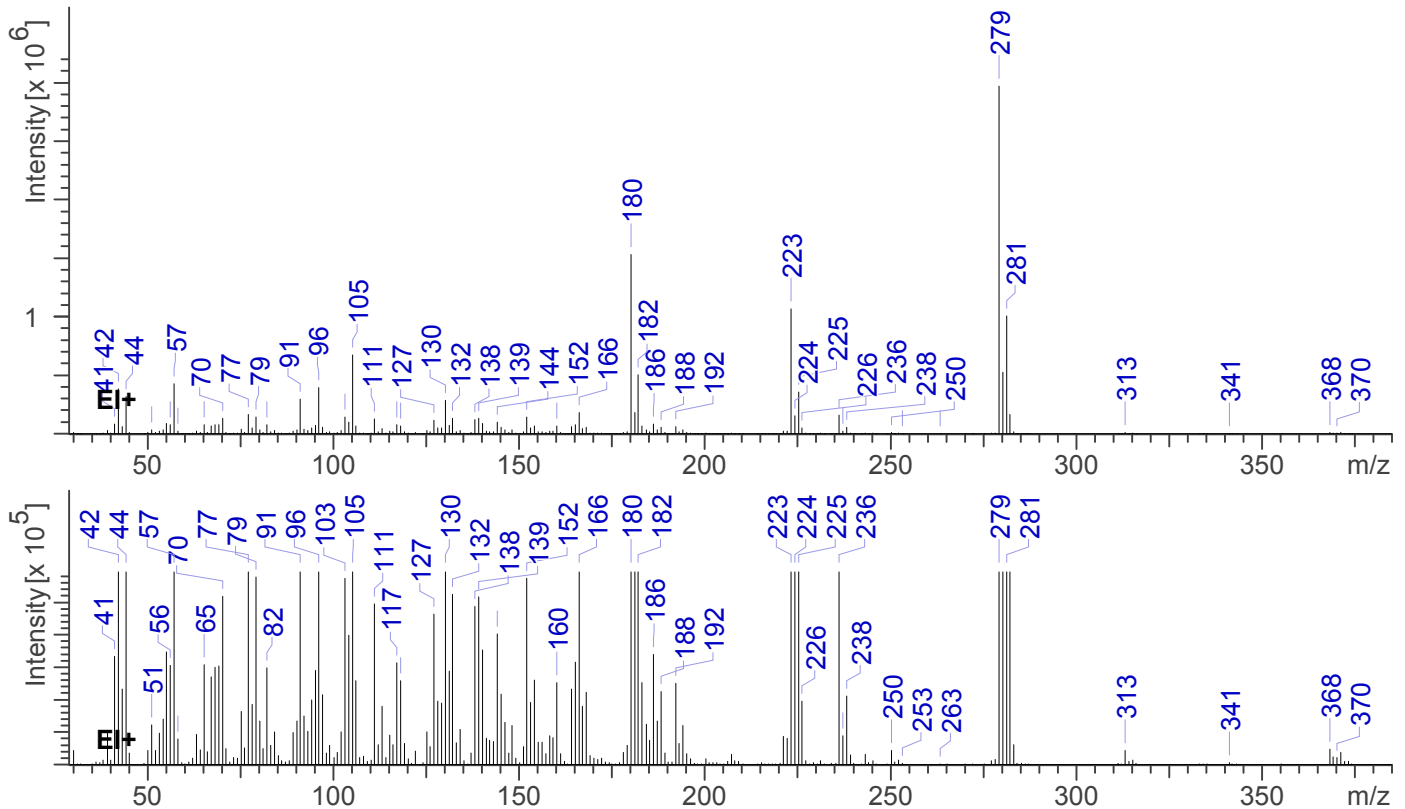
Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

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 1.5mL/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: 17.594min

EI Mass Spectrum: ortho-Chlorofentanyl HCl; Lot# 0600281-13





ortho-Chlorofentanyl



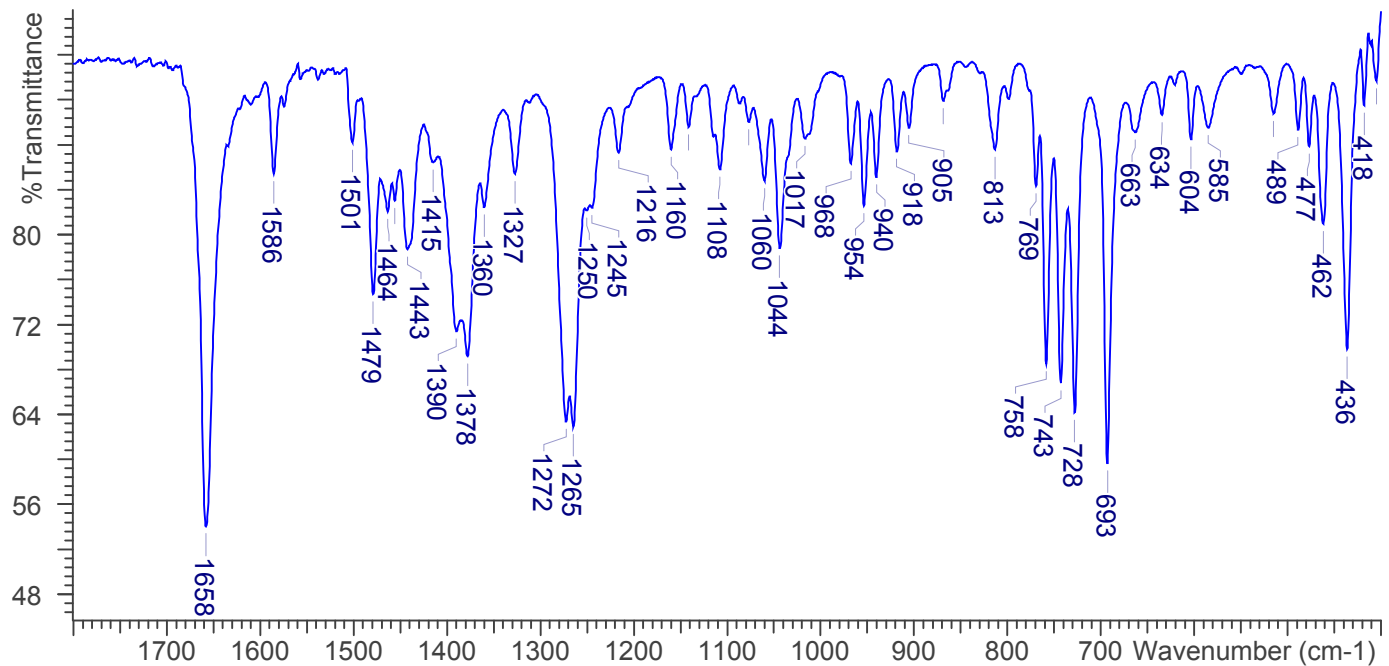
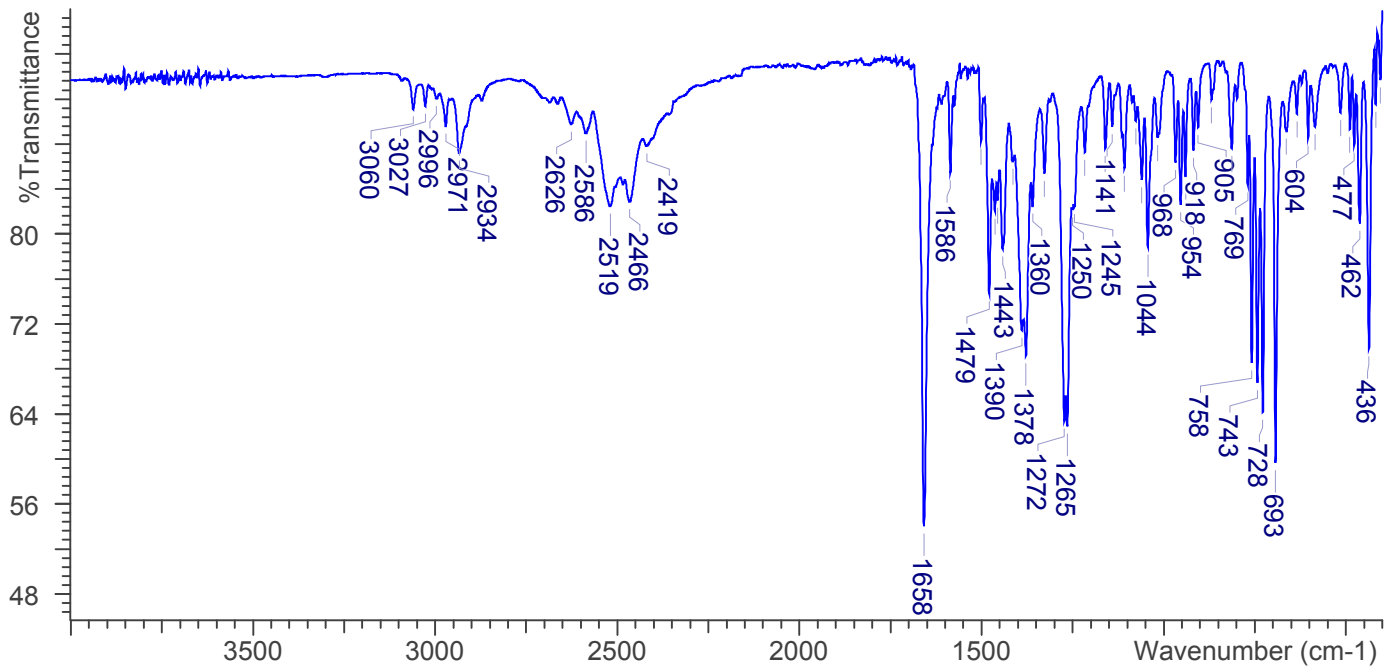
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3.3 INFRARED SPECTROSCOPY (FTIR)

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: 4
Aperture: 150

FTIR ATR (Diamond 1 Bounce): ortho-Chlorofentanyl HCl; Lot# 0600281-13





ortho-Chlorofentanyl



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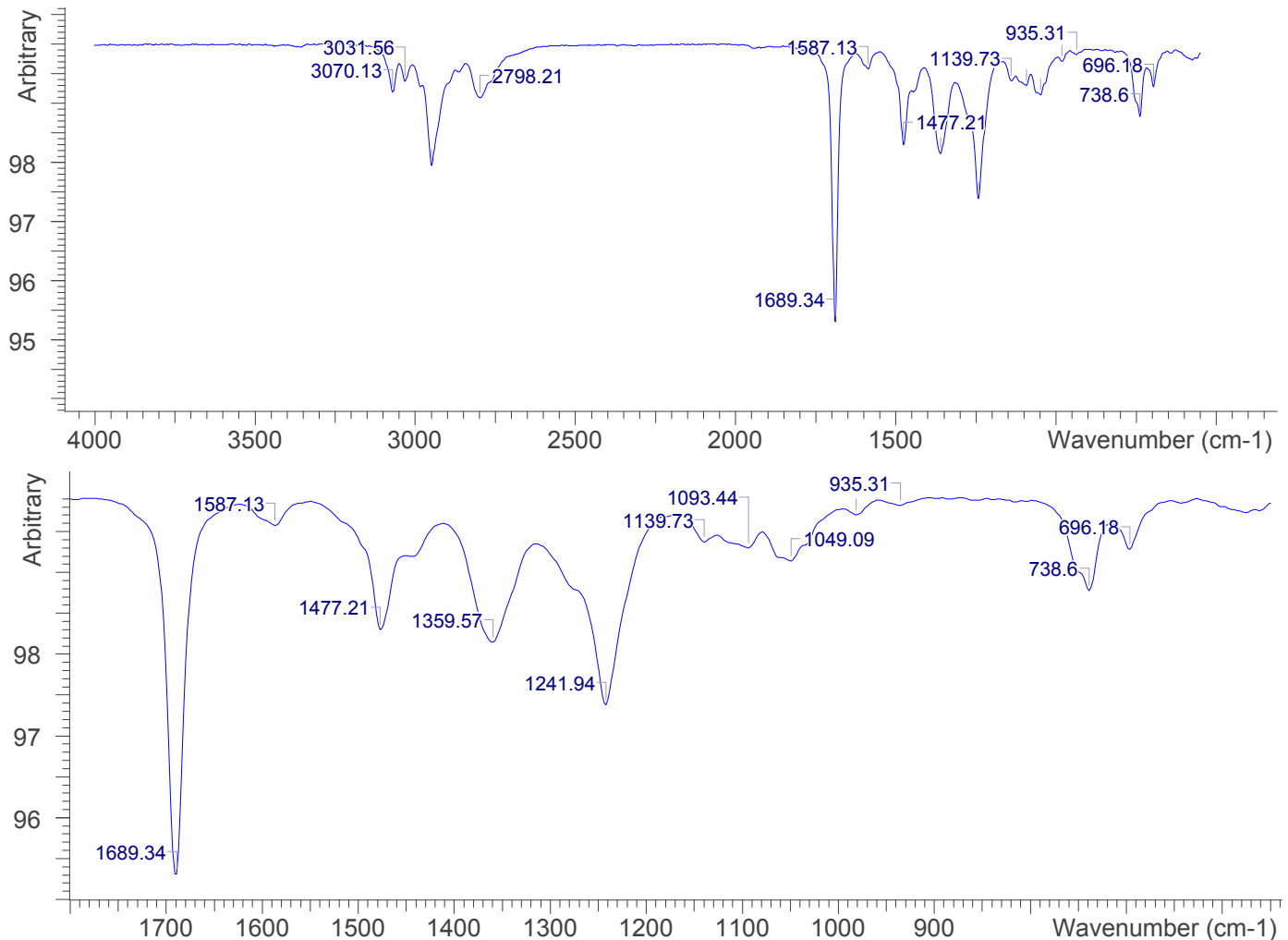
3.4. GAS CHROMATOGRAPHY /INFRARED DETECTION:

Sample Preparation: Dilute analyte 1mg/ml in CHCl₃

Instrument: Gas Chromatograph in split mode with Infrared Detection
Column: HP-5; 30m x 0.32 mm id x 0.25 μm
Carrier Gas: Helium at 2.0mL/min
Temperature: Injector: 280°C Split ratio: 2:1, 2μl injection
65°C hold 1.5min., ramp to 310°C at 20°C/min., hold 5min.

IRD: Detector: Transfer line
Temp 280°C
Flow Cell Temp 280°C
Resolution 8 cm⁻¹

GC-IRD: ortho-Chlorofentanyl HCl; Lot# 0600281-13





ortho-Chlorofentanyl



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4. ADDITIONAL RESOURCES

No additional resources as of 07/16/2021