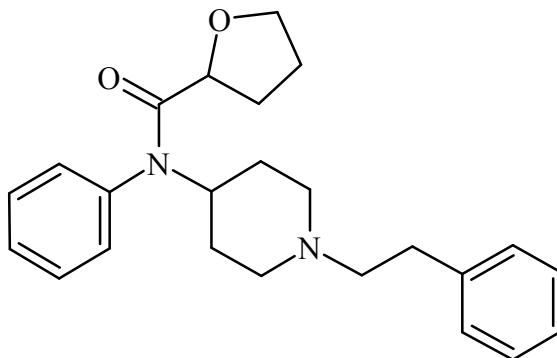




Tetrahydrofuran Fentanyl

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



1. GENERAL INFORMATION

IUPAC Name:	N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]tetrahydrofuran-2-carboxamide
CAS#:	Not available
Synonyms:	THF Fentanyl, Tetrahydrofuranyl Fentanyl, N-(1-phenethylpiperidin-4-yl)-N-phenyltetrahydrofuran-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 ₃₀ N ₂ O ₂	378.51	Not Determined
HCl	C ₂₄ H ₃₀ N ₂ O ₂ HCl	414.97	Not Determined



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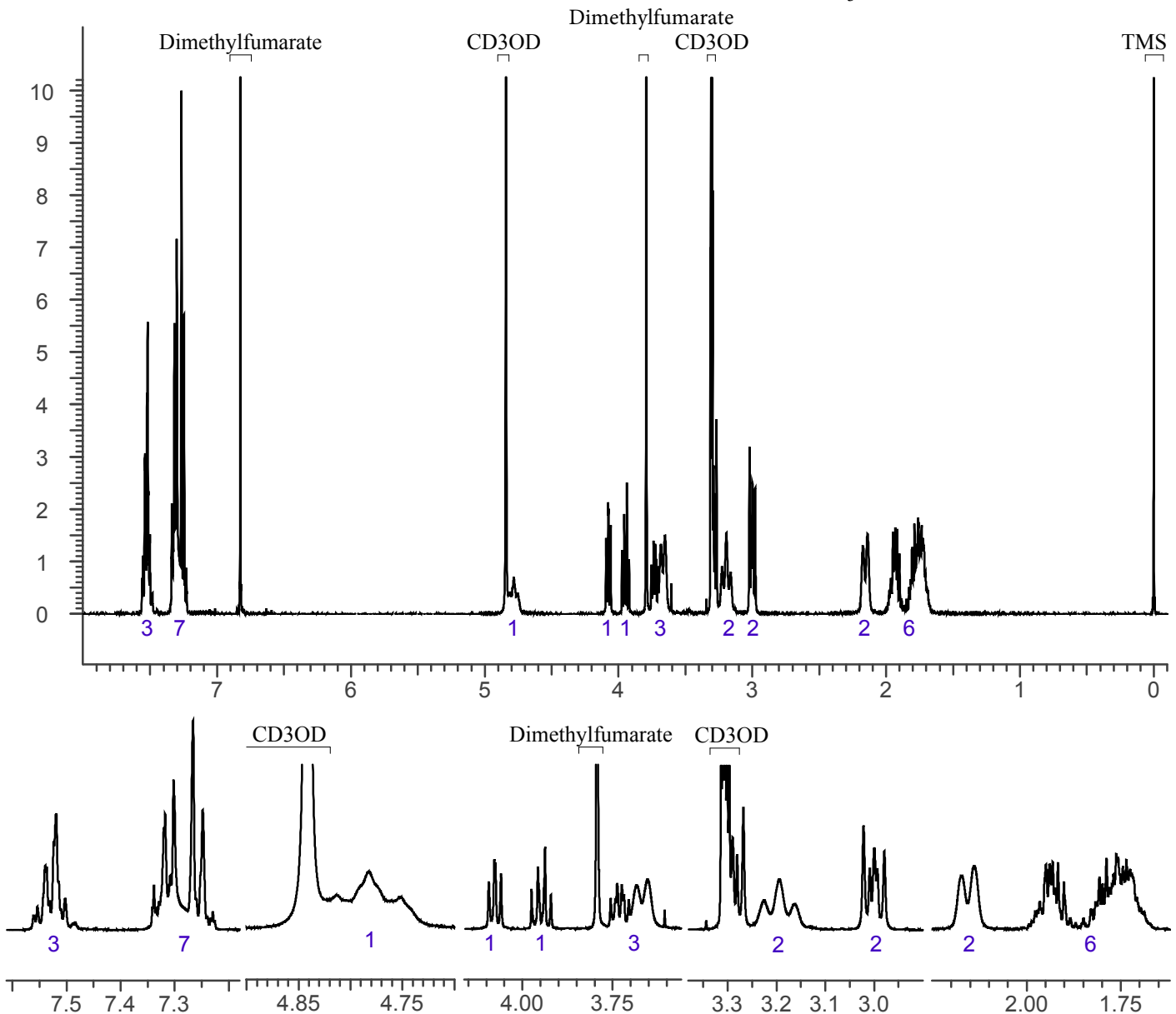
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in CD₃OD 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: Tetrahydrofuran Fentanyl HCl; Lot 0497941-14; CD₃OD; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

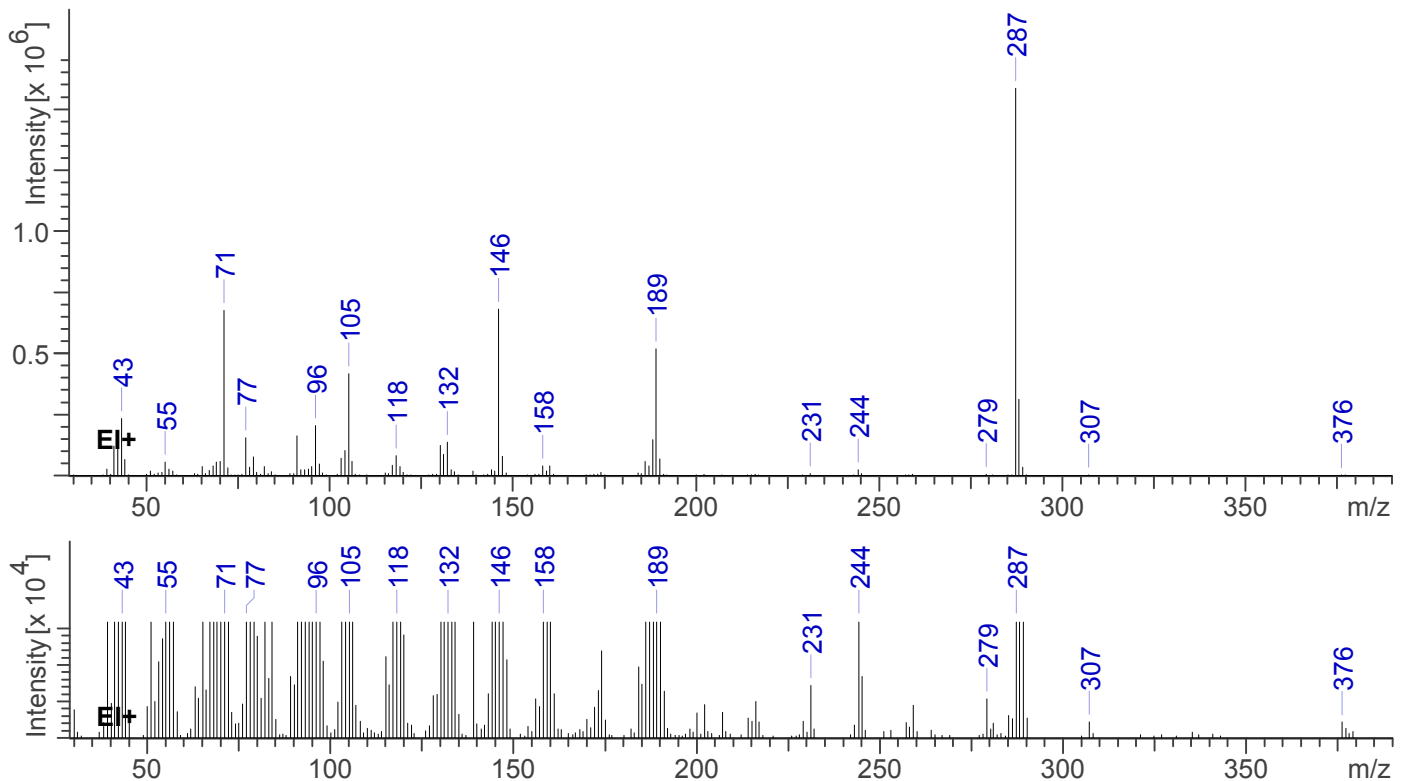
Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃.

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 μm
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 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 20.730 min

EI Mass Spectrum: Tetrahydrofuran Fentanyl HCl; Lot 0497941-14





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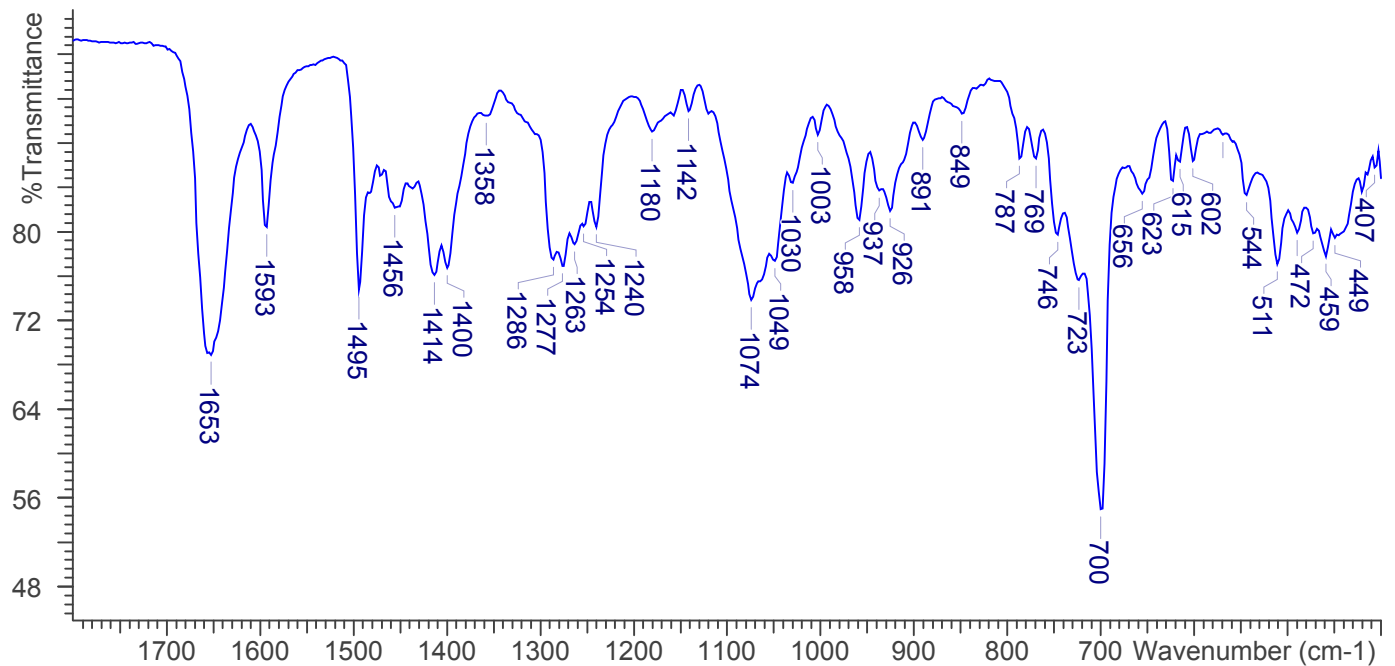
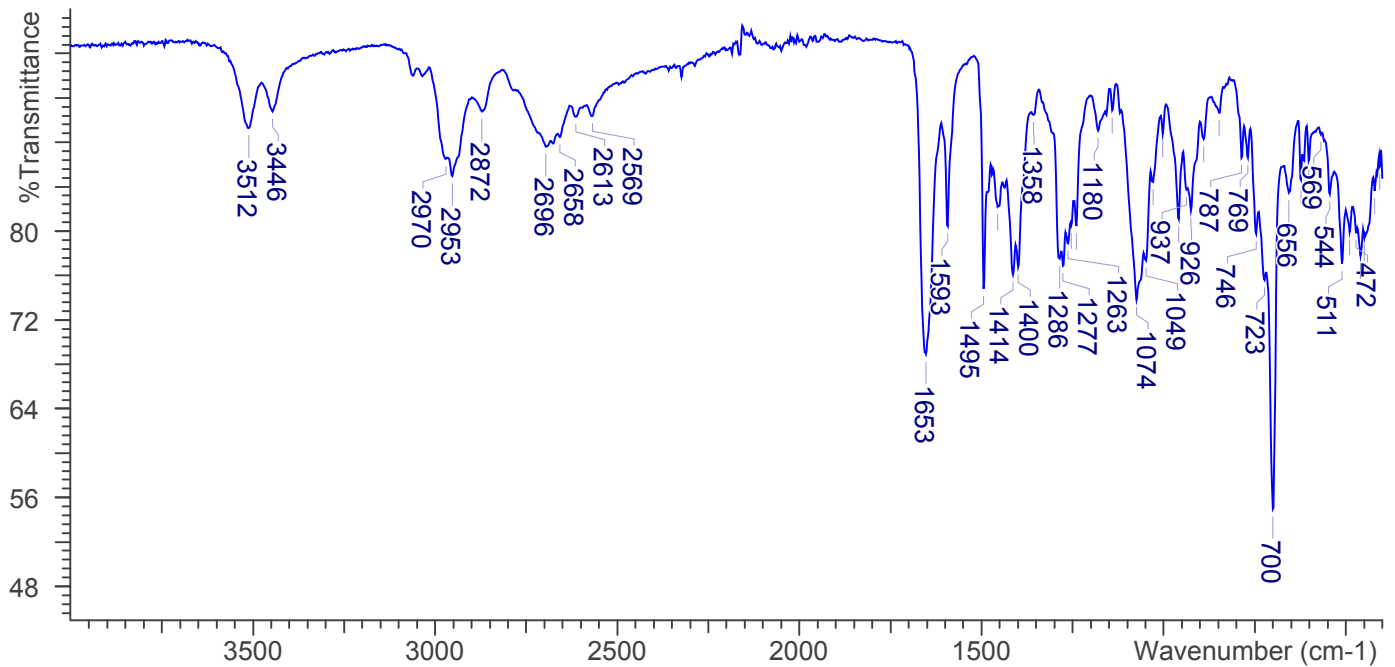


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with Golden Gate ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 16
Number of background scans: 16
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Golden Gate): Tetrahydrofuran Fentanyl HCl; Lot 0497941-14





Tetrahydrofuran Fentanyl

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4. ADDITIONAL RESOURCES

No Literature available as of 06/2017