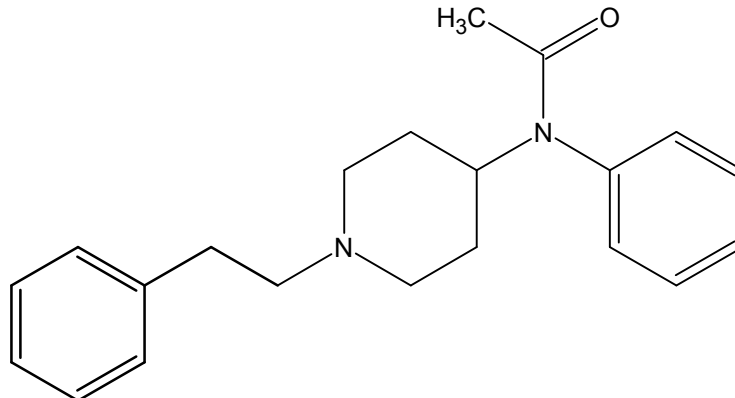




## Acetyl Fentanyl

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	N-[1-(2-phenylethyl)-4-piperidyl]-N-phenylacetamide
<b>CAS#:</b>	3258-84-2
<b>Synonyms:</b>	Fentanyl acetyl analog, N-(1-phenethyl-4-piperidyl)-acetanilide
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	Pale purple powder (HCl)
<b>UV<sub>max</sub>(nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O	322	Not Determined
HCl	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O · HCl	358	256.6



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## 3. QUALITATIVE DATA

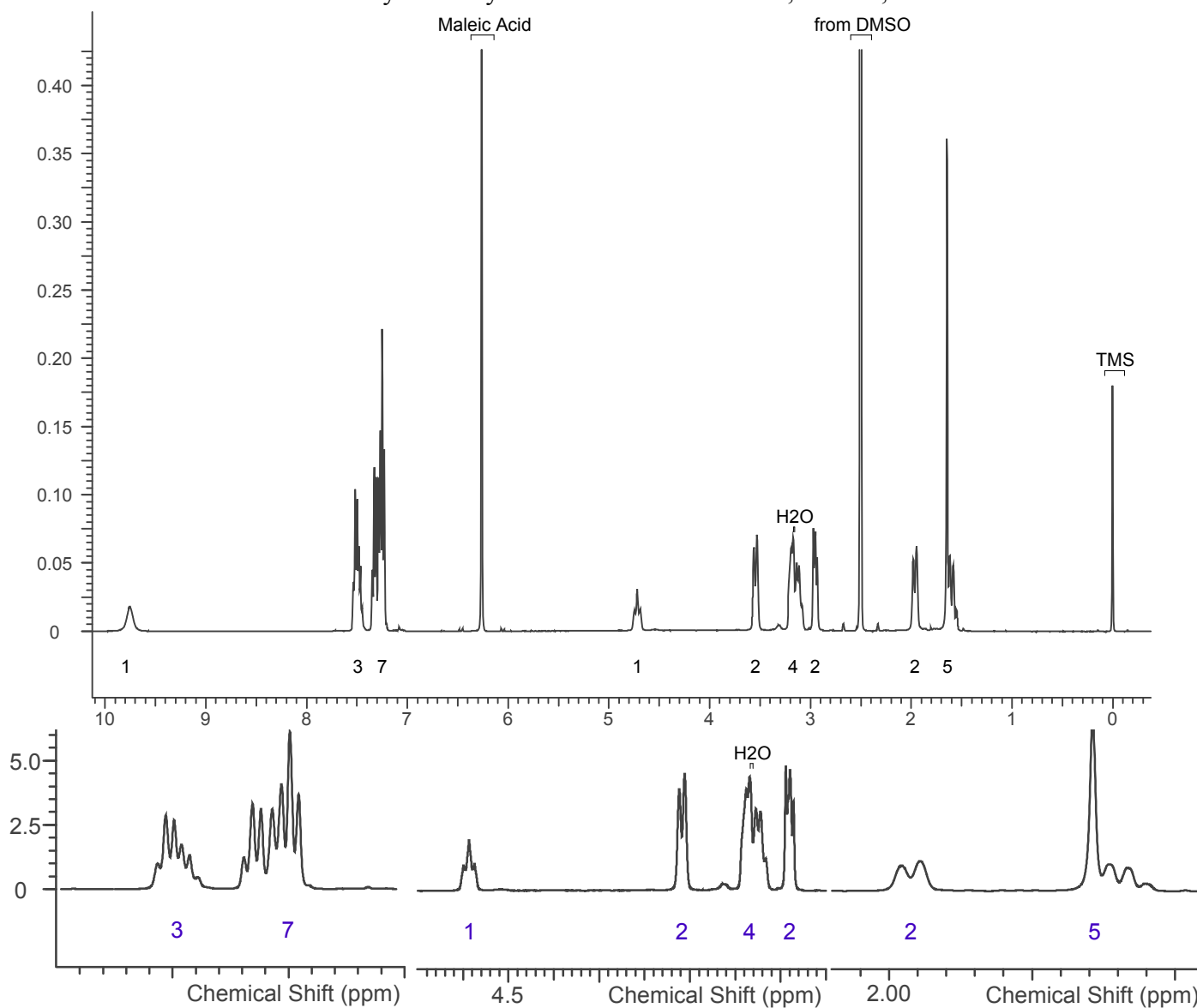
### 3.1 NUCLEAR MAGNETIC RESONANCE

#### Method NMR DMSO

*Sample Preparation:* Dilute analyte to ~5 mg/mL in DMSO containing TMS for 0 ppm reference and maleic acid 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

<sup>1</sup>H NMR: Acetyl Fentanyl HCl Lot 4541-886-149A; DMSO; 400MHz





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## 3.2 Gas Chromatography/Mass Spectrometry

**Sample Preparation:** Dilute analyte ~1 mg/mL in chloroform.

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector

**Column:** DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25  $\mu$ 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 300°C at 12 °C/min

3) Hold final temperature for 9.0 min

**Injection Parameters:** Split Ratio = 20:1, 1  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu

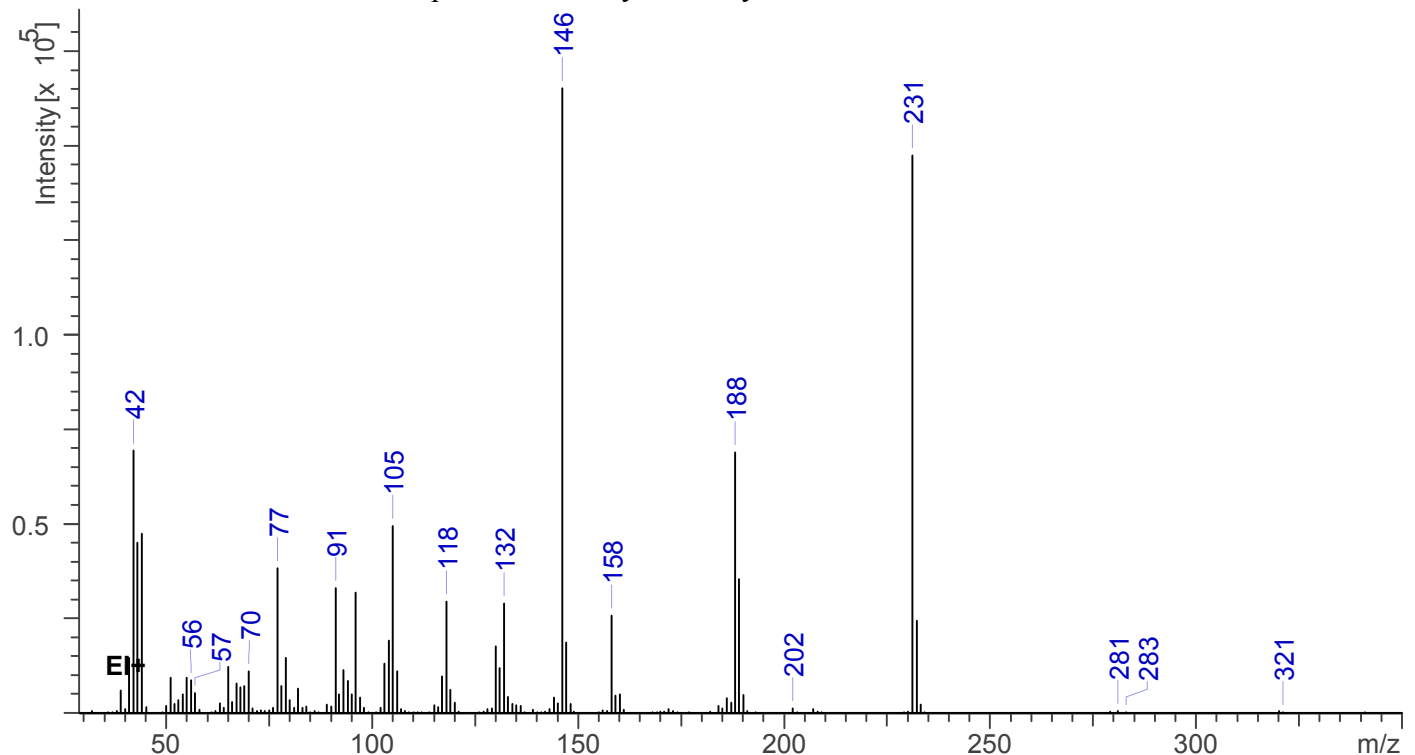
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 16.843 min

EI Mass Spectrum: Acetyl Fentanyl HCl Lot # 4541-886-149A





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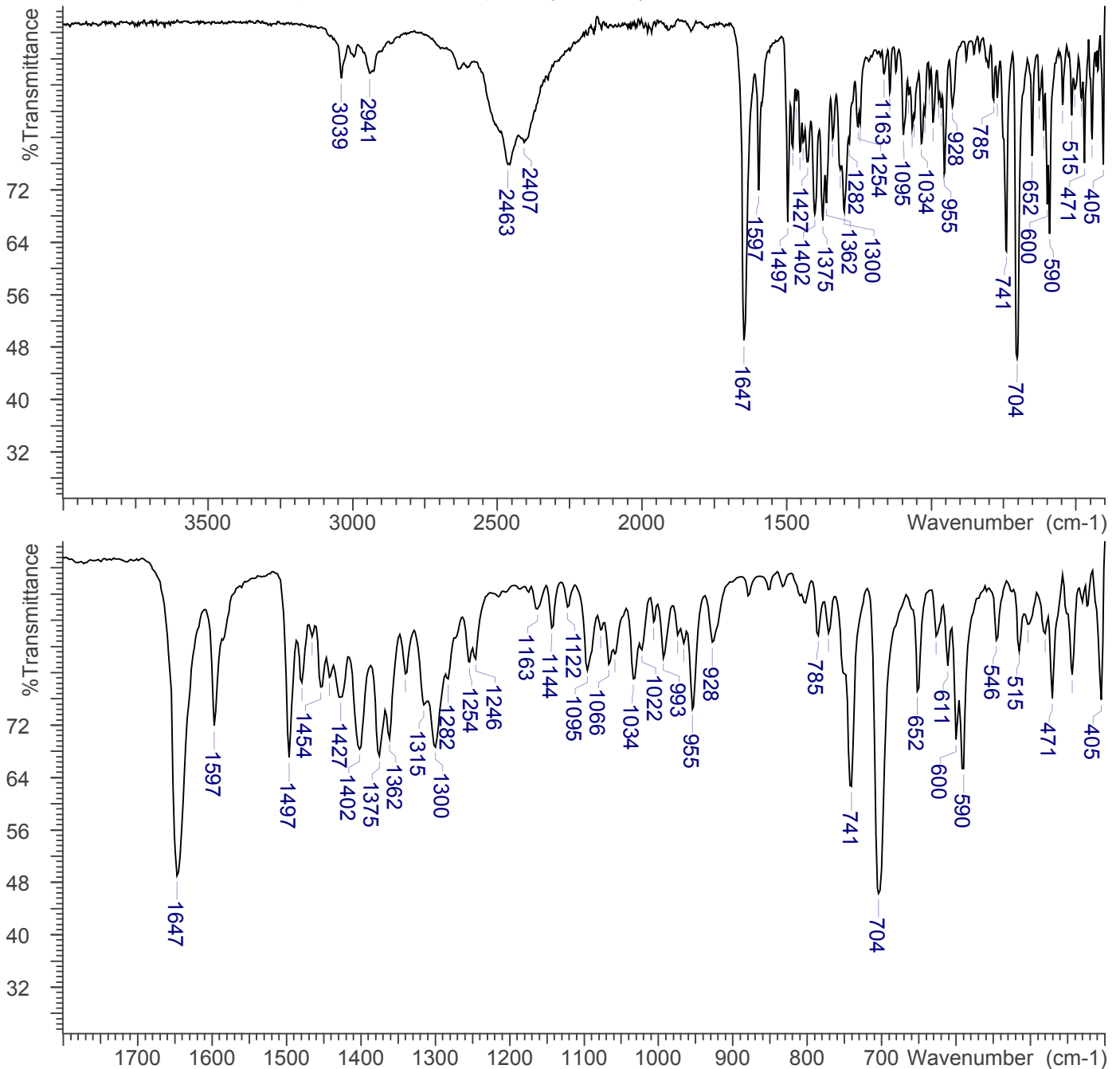


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): Acetyl Fentanyl HCl Lot # 4541-886-149A





## Acetyl Fentanyl

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### **4. ADDITIONAL RESOURCES**

Brine G.A., Boldt K.G., Huang P.T., Sawyer D.K., Carroll F.I. Carbon-13 Nuclear Magnetic Resonance Spectra of Fentanyl Analogs. *J. Heterocyclic Chem.* 1989; 26: 677-686.