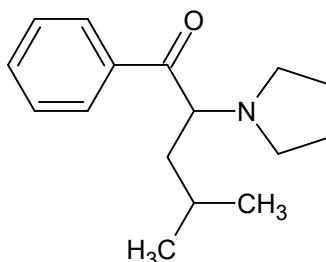




## 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one

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>	4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one
<b>CAS#:</b>	N/A
<b>Synonyms:</b>	N/A
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<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>16</sub> H <sub>23</sub> NO	245.36	Not Determined
HCl	C <sub>16</sub> H <sub>23</sub> NO HCl	281.82	Not Determined



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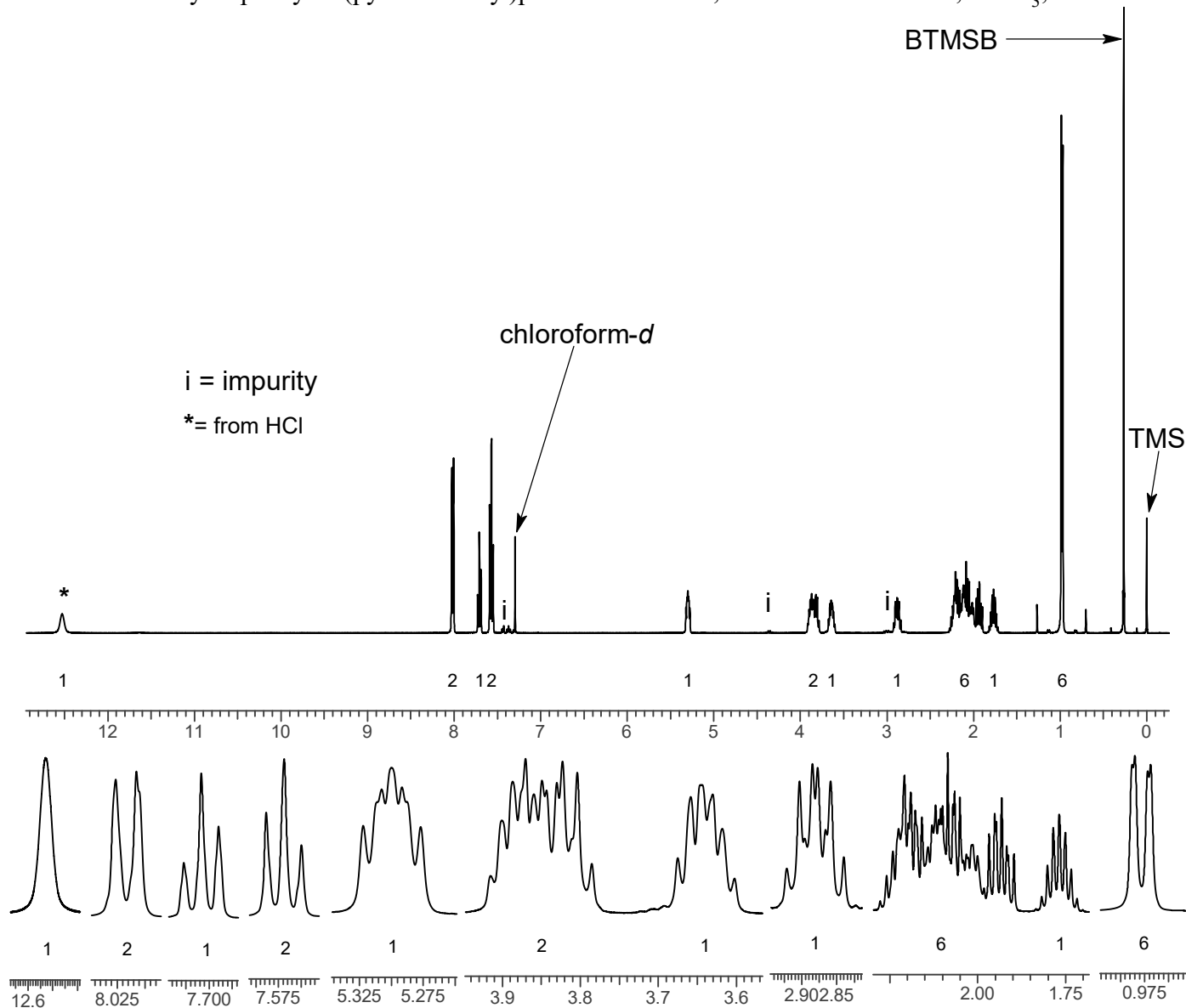
### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~19 mg/mL in CDCl<sub>3</sub> containing TMS for 0 ppm reference and 1,4-BTMSB-*d*<sub>4</sub> 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>HNMR: 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one HCl; Lot# RM-161101-01; CDCl<sub>3</sub>; 400MHz





## 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~3 mg/mL in CHCl<sub>3</sub>

**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

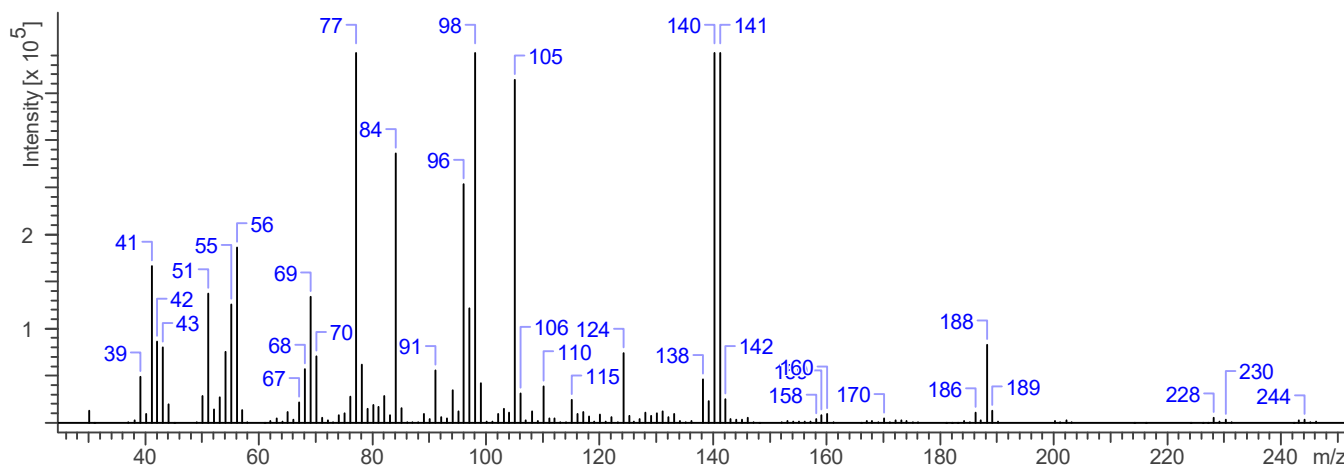
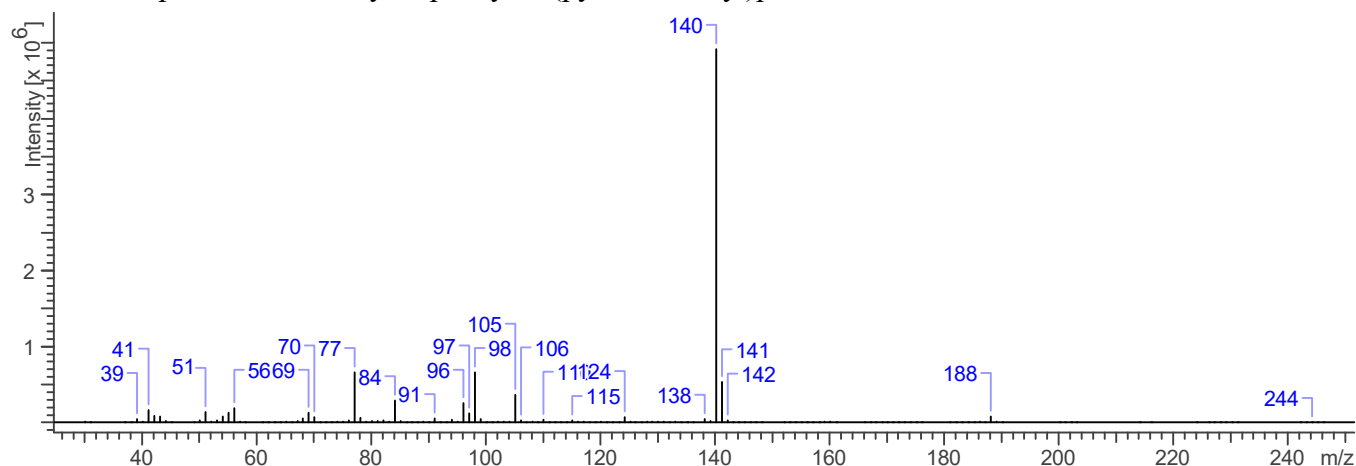
**Injection Parameters:** Split Ratio = 25:1, 1 μL injected

**MS Parameters:** Mass scan range: 30-550 amu                      Threshold: 250

Tune file: stune.u                      Acquisition mode: scan

**Retention Time:** 9.92 min

EI Mass Spectrum: 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one HCl; Lot# RM-161101-01





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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<sup>-1</sup>  
Sample gain: 1  
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one HCl; Lot# RM-161101-01

