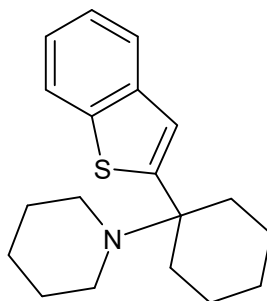




## Benocyclidine

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>           | 1-[1-(1-benzothiophen-2-yl)cyclohexyl]piperidine     |
| <b>CAS#:</b>                 | 112726-66-6  |
| <b>Synonyms:</b>             | BCP, BTCP, GK13, Benzothiophenylcyclohexylpiperidine |
| <b>Source:</b>               | DEA Reference Material Collection                    |
| <b>Appearance:</b>           | Yellow 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>19</sub> H <sub>25</sub> NS | 299.47           | Not Determined     |



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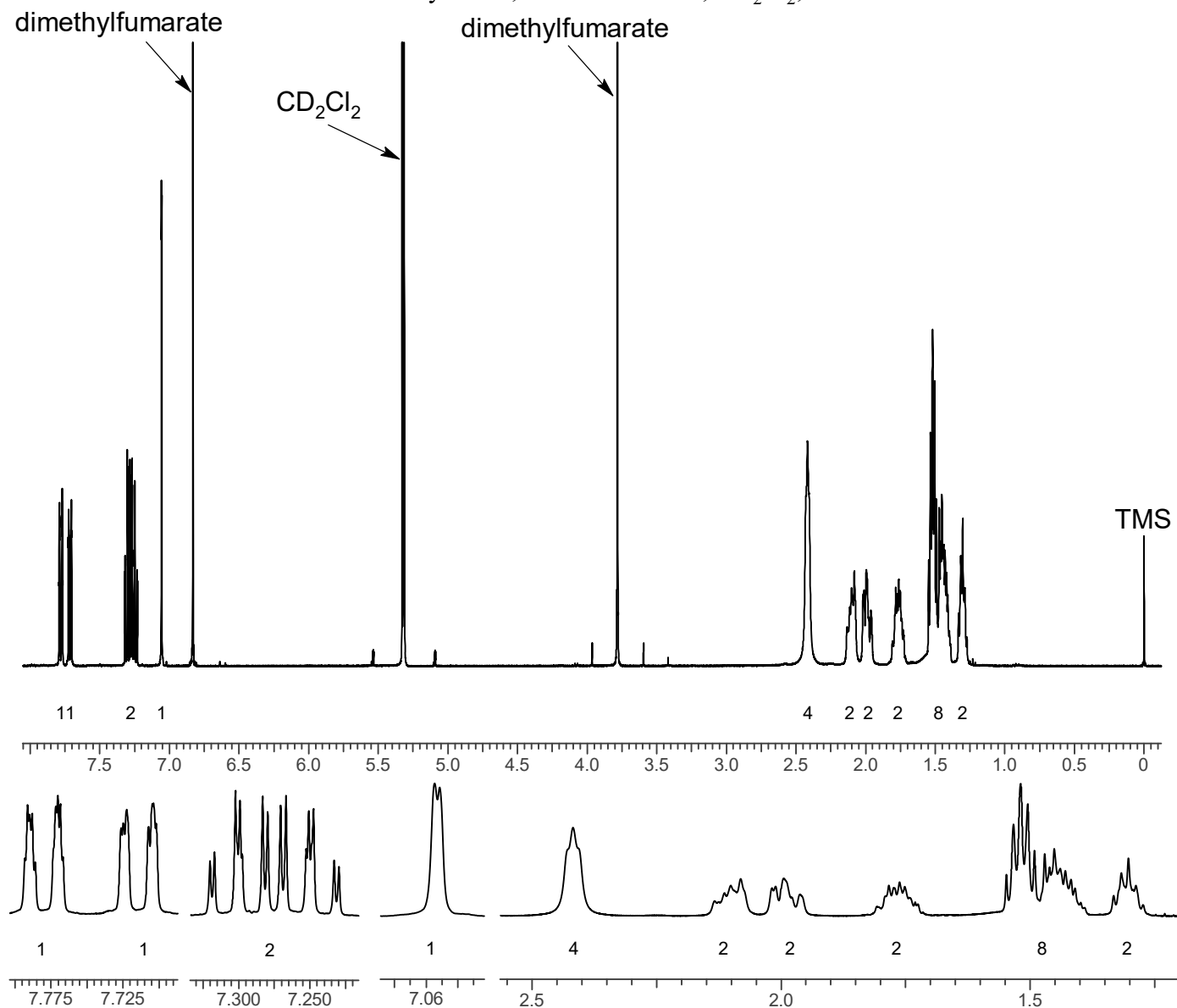
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in  $CD_2Cl_2$  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:  $90^\circ$   
Delay between pulses: 45 seconds

$^1H$ NMR: Benocyclidine; Lot# 0546715-1;  $CD_2Cl_2$ ; 400MHz





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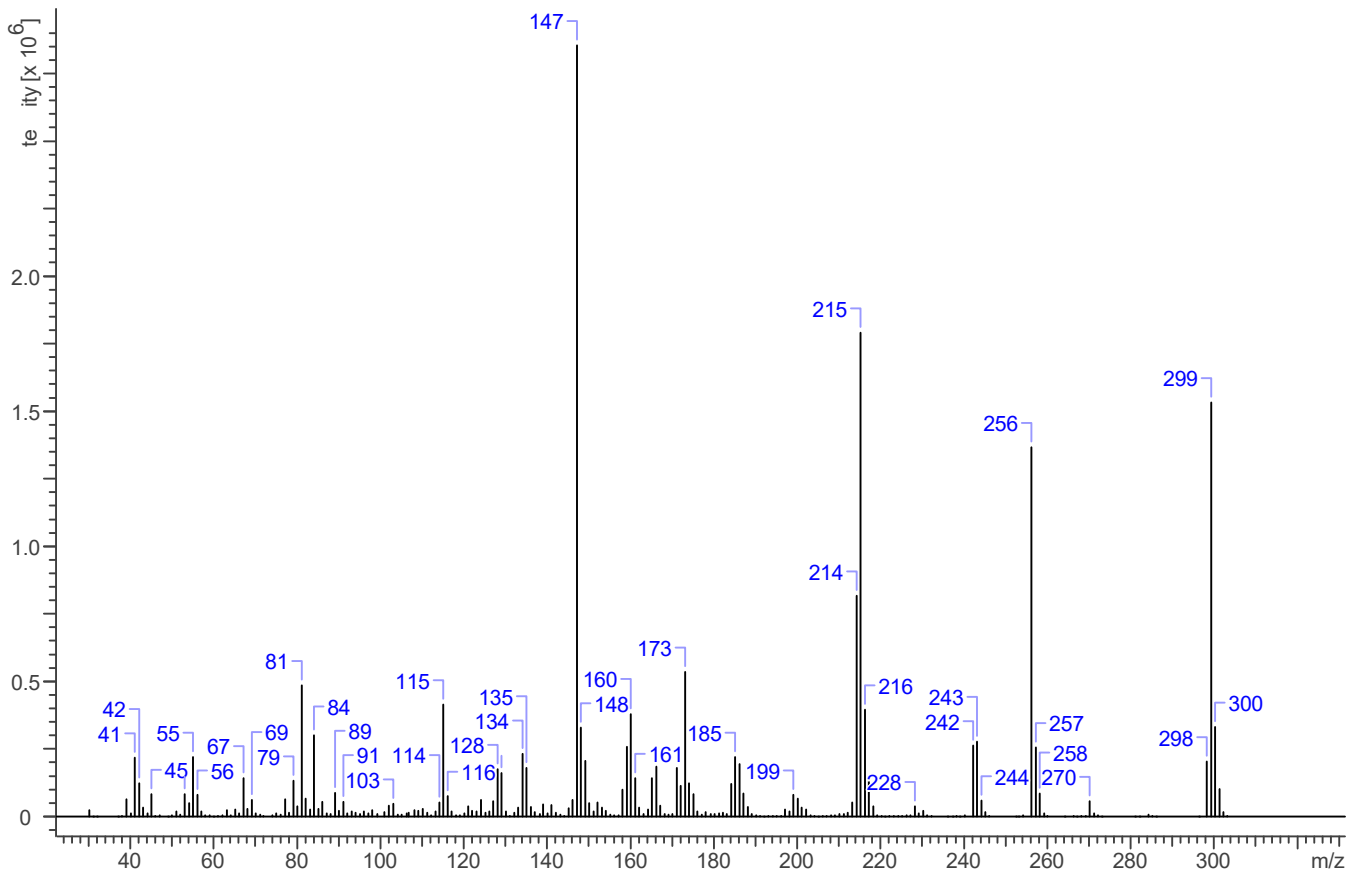


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~7 mg/2mL in 1:1 CHCl<sub>3</sub>:MeOH

**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:** 14.93 min

EI Mass Spectrum: Benocyclidine; Lot# 0546715-1





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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: 1  
Aperture: 150

FTIR ATR (Diamond 3 Bounce): Benocyclidine; Lot# 0546715-1

