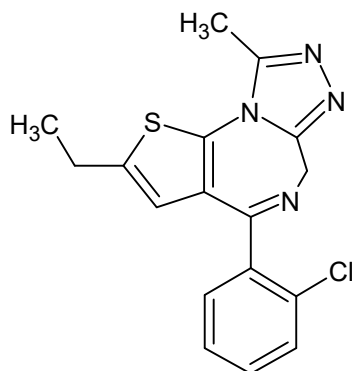




# Etizolam

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



## 1. GENERAL INFORMATION

**IUPAC Name:** 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine

**CAS#:** 40054-69-1

**Synonyms:** NA

**Source:** DEA Reference Material Collection

**Appearance:** White Powder

**UV<sub>max</sub>(nm):** Not determined

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Neutral	C <sub>17</sub> H <sub>15</sub> ClN <sub>4</sub> S	342	142.8



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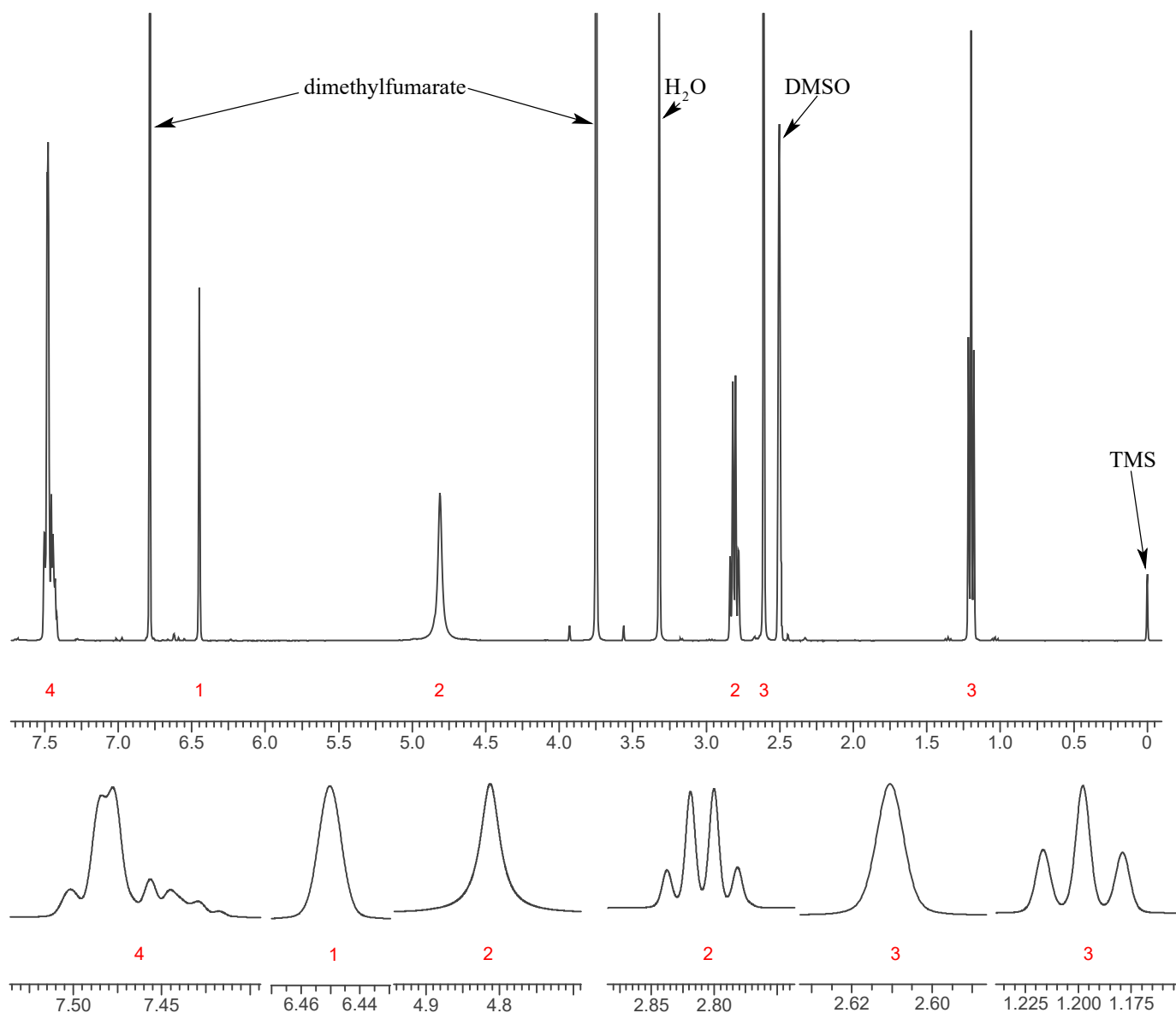
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~9 mg/mL in DMSO- $d_6$  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

$^1\text{H}$ NMR: Etizolam; Lot# 17313; DMSO- $d_6$ ; 400MHz





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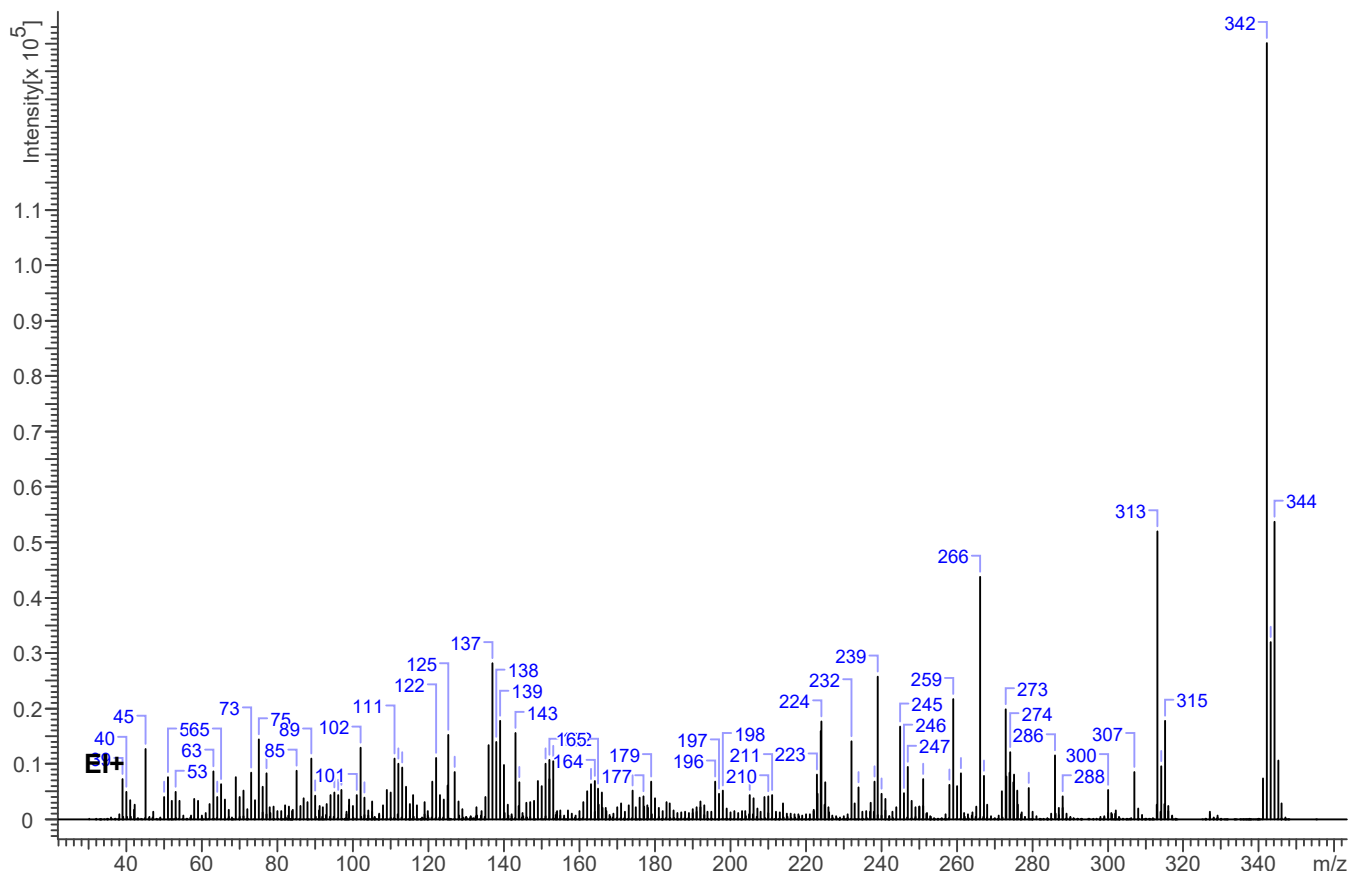


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~4 mg/mL in CHCl<sub>3</sub>

**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 μm  
**Carrier Gas:** Helium at 1.0 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 μL injected  
**MS Parameters:** Mass scan range: 30-550 amu                      Threshold: 100  
Tune file: stune.u                      Acquisition mode: scan  
**Retention Time:** 18.013 min

EI Mass Spectrum: Etizolam; Lot# 17313





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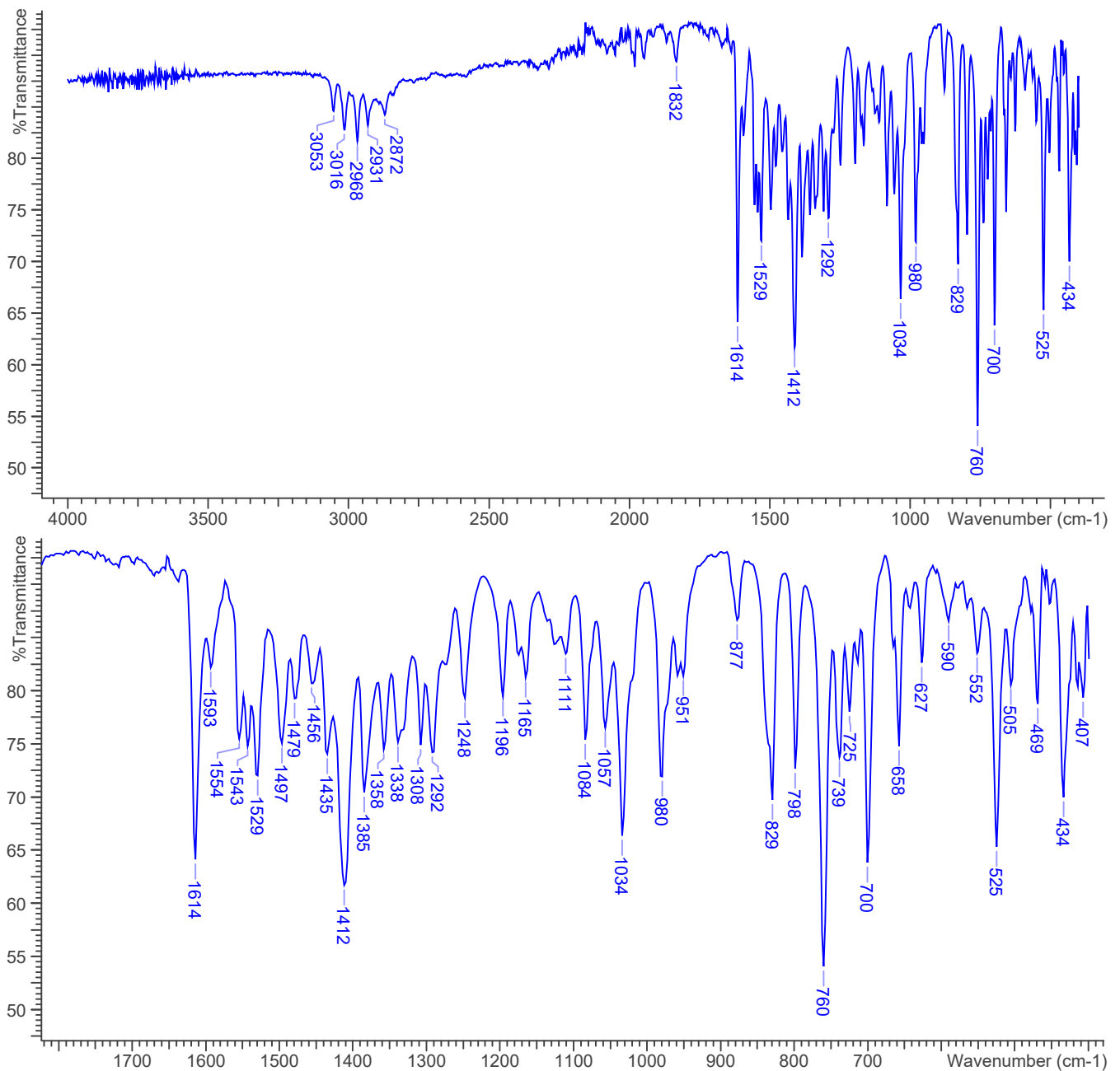


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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: 8  
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Etizolam; Lot# 17313





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### **4. ADDITIONAL RESOURCES**

[\*Wikipedia\*](#)

[\*Forendex\*](#)