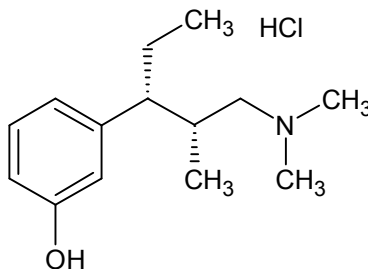




# Tapentadol

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



## 1. GENERAL INFORMATION

**IUPAC Name:** *rel*-3-[(2*R*,3*R*)-1-(dimethylamino)-2-methylpentan-3-yl]phenol

**CAS#:** 175591-09-0 (HCl)

**Synonyms:** Nucynta, Palexia, Tapal

**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)
Base	C <sub>14</sub> H <sub>23</sub> NO	221	Not Determined
HCl	C <sub>14</sub> H <sub>23</sub> NO HCl	257	Not Determined



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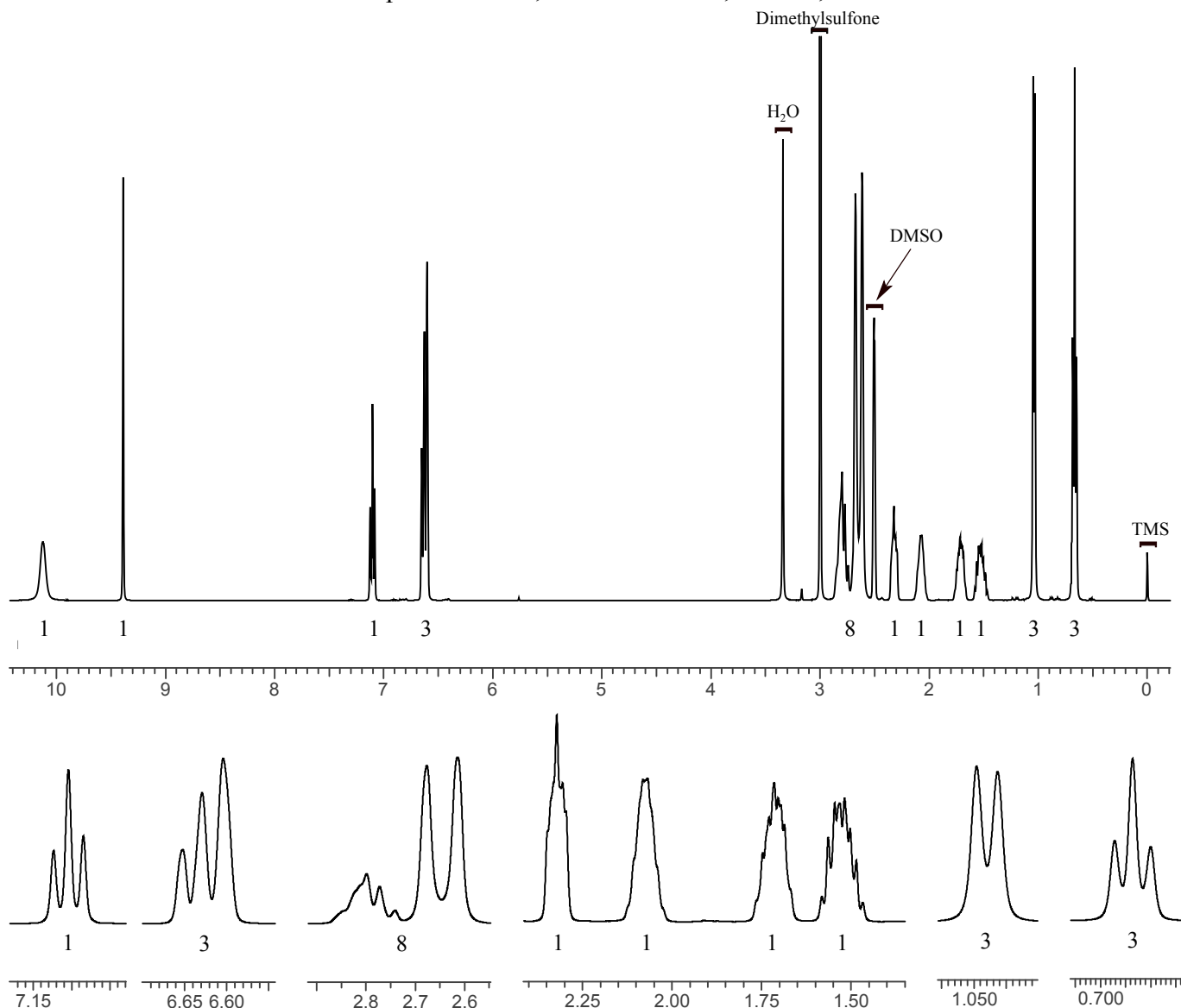
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in DMSO- $d_6$  containing TMS for 0 ppm reference and dimethylsulfone 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: Tapentadol HCl; Lot 1665.1B1.1; DMSO; 400MHz





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## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

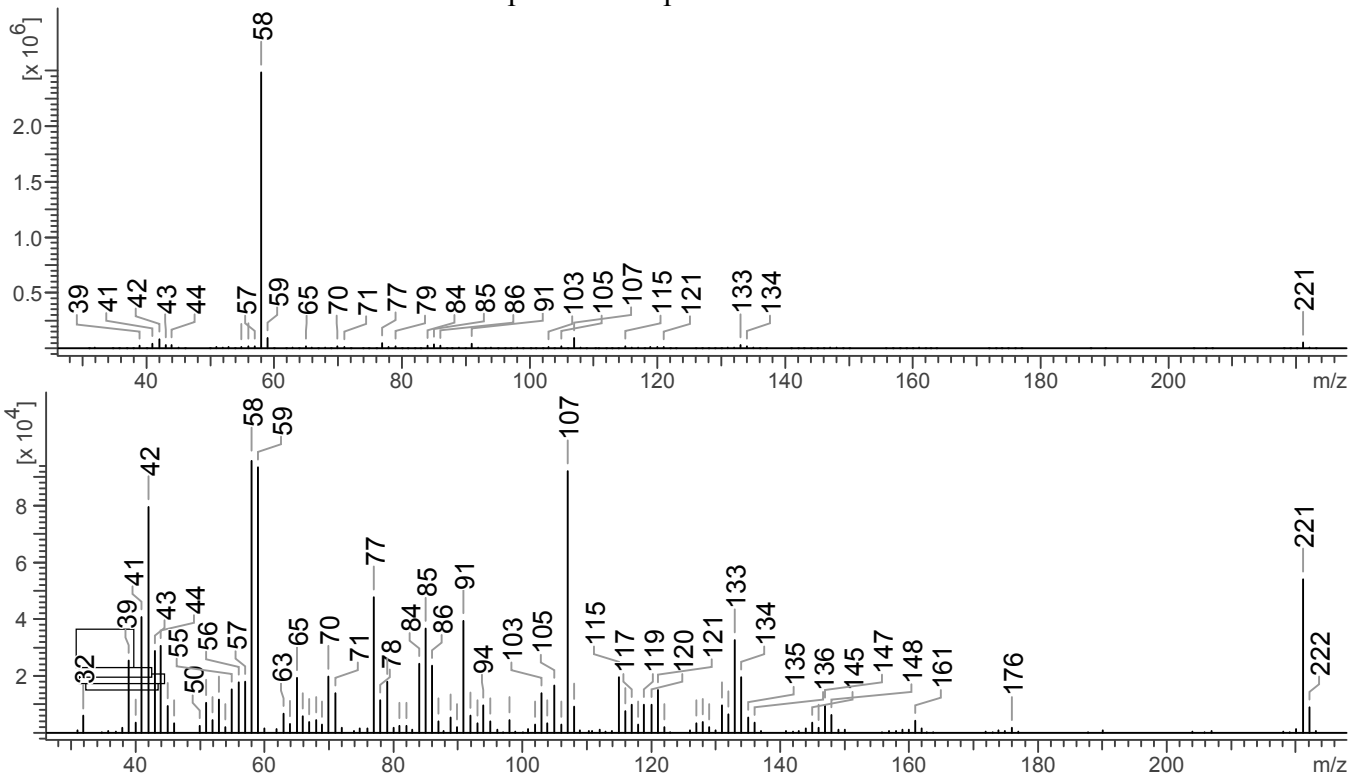
**Sample Preparation:** Dilute analyte ~4.8 mg/mL in 1:1 CHCl<sub>3</sub>: MeOH

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** DB-5 MS (or equivalent); 15m 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: 250°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: 150  
Tune file: stune.u  
Acquisition mode: scan

**Retention Time:** 6.73 min

EI Mass Spectrum: Tapentadol HCl Lot 1665.1B1.1





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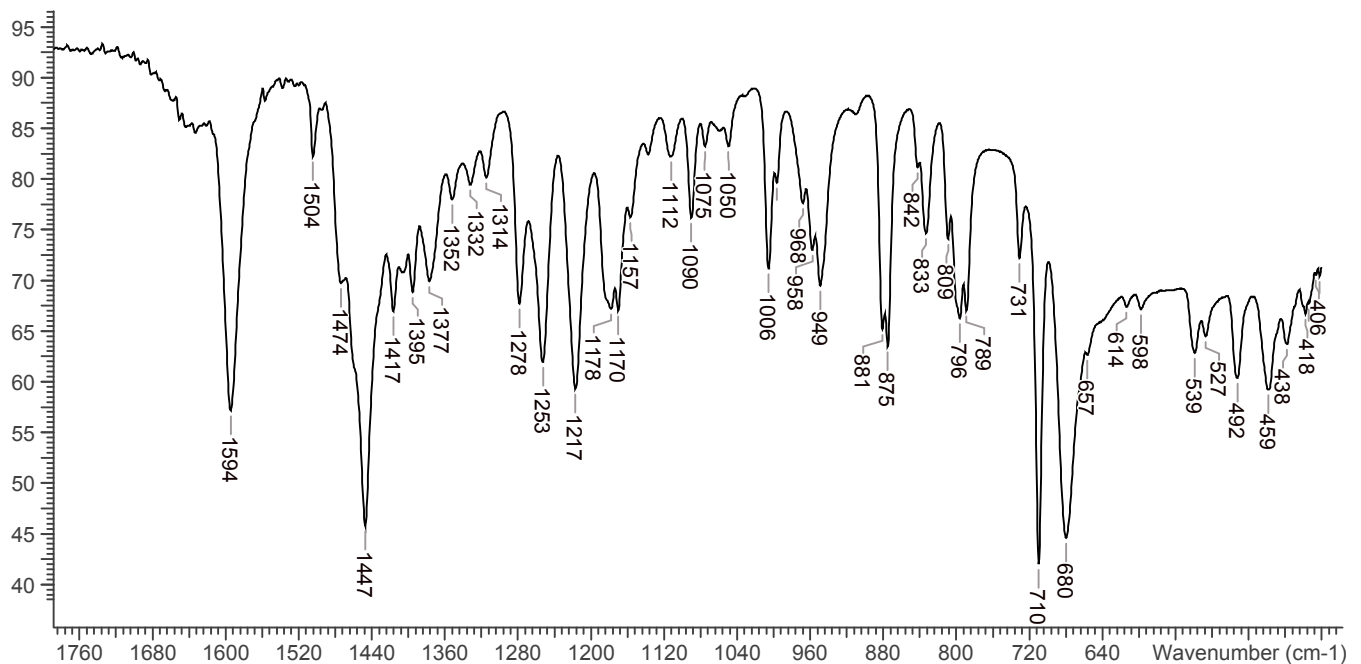
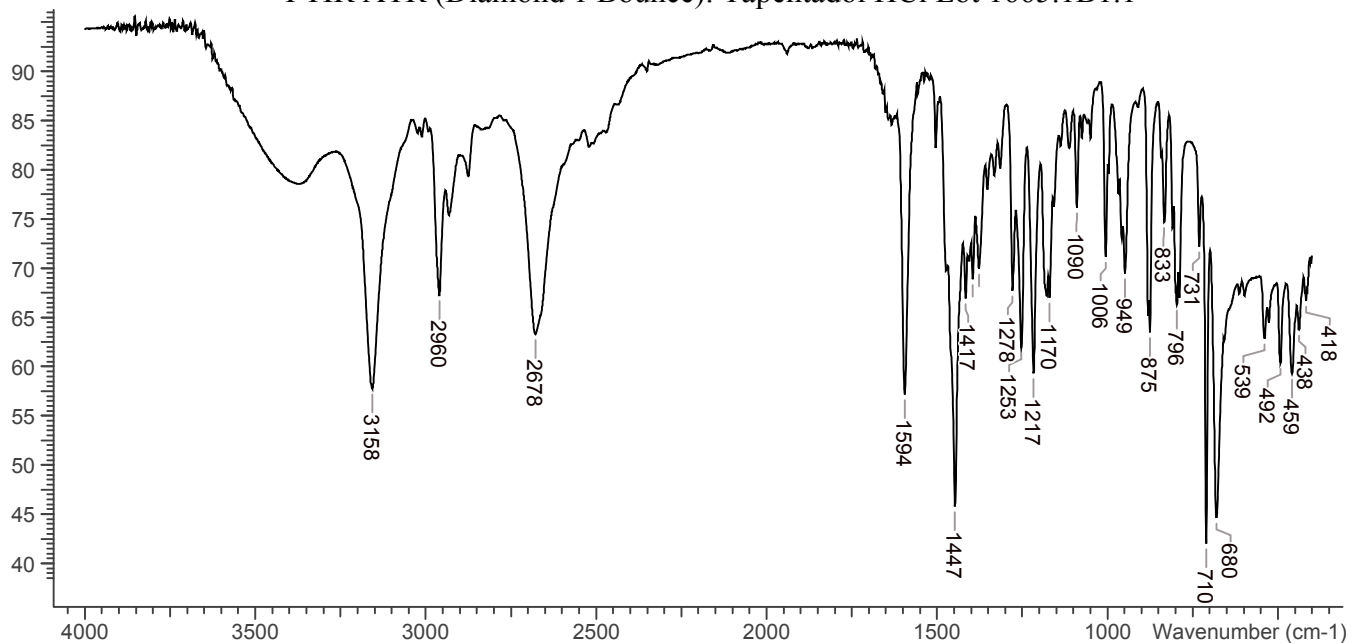


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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): Tapentadol HCl Lot 1665.1B1.1





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### 4. ADDITIONAL RESOURCES

[\*Wikipedia\*](#)

[\*Forendex\*](#)