1. GENERAL INFORMATION

**IUPAC Name:** 2-(pyrrolidin-1-yl)-1-(5,6,7,8-tetrahydroxanaphthalen-2-yl)pentan-1-one

**CAS#:** NA

**Synonyms:** 1-(5,6,7,8-tetrahydroxanaphthalen-2-yl)-2-(pyrrolidin-1-yl)pentan-1-one; 3',4'-tremethylene- α-pyrrolidinovalerophenone; 3',4'-tremethylene- α-PVP

**Source:** DEA Reference Material Collection

**Appearance:** White Powder

**UV\_max (nm):** Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C\textsubscript{19}H\textsubscript{27}NO</td>
<td>285</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{19}H\textsubscript{27}NO HCl</td>
<td>322</td>
<td>256.8</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~15 mg/mL in CDCl$_3$ 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

$^1$HNMR: TH-PVP HCl; Lot # RM-160223-02; CDCl$_3$; 400MHz

![NMR Spectroscopy Diagram]
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃ after base extraction with NaOH

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 0.9 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: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 14.614 min

EI Mass Spectrum: TH-PVP HCl; Lot # RM-160223-02
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⁻¹
- Sample gain: 1
- Aperture: 150

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

FTIR ATR (Diamond 1 Bounce): TH-PVP HCl; Lot # RM-160223-02
4. ADDITIONAL RESOURCES

No additional resources as of 03/2016