Mexedrone

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

1. GENERAL INFORMATION

IUPAC Name: 3-methoxy-2-(methylamino)-1-(4-methylphenyl)propan-1-one

CAS#: NA

Synonyms: NA

Source: DEA Reference Material Collection

Appearance: White Powder (HCl)

UV\text{max}\,(\text{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>$\text{C}<em>{12}\text{H}</em>{17}\text{NO}_2$</td>
<td>207</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>$\text{C}<em>{12}\text{H}</em>{17}\text{NO}_2\text{HCl}$</td>
<td>243</td>
<td>193.0-194.1</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

*Sample Preparation:* Dilute analyte to ~26 mg/mL in D$_2$O containing TSP for 0 ppm reference and maleic acid 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: Mexedrone HCl; Lot# RM-160203-01; D$_2$O; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~4 mg/mL in CHCl₃ (sample base extracted)

**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:** 6.14 min

**EI Mass Spectrum:** Mexedrone HCl; Lot# RM-160203-01
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
- Sample gain: 1
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): Mexedrone HCl; Lot# RM-160203-01
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4. ADDITIONAL RESOURCES

Wikipedia

Forendex