1. GENERAL INFORMATION

**IUPAC Name:** 1-(3-chlorophenyl)-2-(dimethylamino)propan-1-one

**CAS#:** 514168-22-0 (HCl)

**Synonyms:** 3-Cl-N,N-DMC, 3-Chloro-N,N-DMC

**Source:** Cayman Chemical

**Appearance:** White powder

**UV<sub>max</sub>(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&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;14&lt;/sub&gt;CINO</td>
<td>211.69</td>
<td>N/A</td>
</tr>
<tr>
<td>Hydrochloride</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;14&lt;/sub&gt;CINO HCl</td>
<td>248.15</td>
<td>N/A</td>
</tr>
</tbody>
</table>
3-Chloro-N,N-Dimethylcathinone

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

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 dimethyl sulfoxide 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: 3-Chloro-N,N-Dimethylcathinone HCl; Lot 0533202-18; D$_2$O; 400 MHz

![NMR Spectrogram]
3-Chloro-N,N-Dimethylcathinone

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~3mg/mL in CHCl₃, base extracted.

**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: 100
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 6.904 min

**EI Mass Spectrum:** 3-Chloro-N,N-Dimethylcathinone; Lot#0533202-18

Ion Mode: EI+
3-Chloro-N,N-Dimethylcathinone

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3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** Scan FTIR with diamond ATR attachment (1 bounce)

**Parameters:**
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 4.0
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): 3-Chloro-N,N-Dimethylcathinone; Lot# 0533202-18