1. GENERAL INFORMATION

**IUPAC Name:** 2-(3,4-dichlorophenyl)-N-(2-(dimethylamino)cyclohexyl)-N-methylacetamide

**CAS#:** N/A

**Synonyms:** trans-3,4-dichloro-N-[2-(dimethylamino)cyclohexyl]-N-methylbenzenacetamide

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**$UV_{\text{max}}$ (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>$\text{C}<em>{17}\text{H}</em>{24}\text{Cl}_2\text{N}_2\text{O}$</td>
<td>343.29</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>$\text{C}<em>{17}\text{H}</em>{24}\text{Cl}_2\text{N}_2\text{O} \cdot \text{HCl}$</td>
<td>379.75</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
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 maleic acid as quantitative internal standard.

**Instrument:** 400 MHz NMR spectrometer

**Parameters:**
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: $90^\circ$
- Delay between pulses: 45 seconds

$^1$HNMR: U-51754 HCl; Lot# 0505031-15; DMSO-$d_6$; 400MHz

![NMR spectrum of U-51754](image)

NH

maleic acid

DMSO

TMS

Latest Revision: 2/8/2019 SWGDRUG.org/monographs.htm
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

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:
- 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
- Injector: 280°C
- MSD transfer line: 280°C
- MS Source: 230°C
- MS Quad: 150°C

Injection Parameters: Split Ratio = 25:1, 1 μL injected
MS Parameters:
- Mass scan range: 30-550 amu
- Tune file: stune.u
- Acquisition mode: scan
- Threshold: 150

Retention Time: 15.91 min

EI Mass Spectrum: U-51754 HCl; Lot# 0505031-15
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

FTIR ATR (Diamond 1 Bounce): U-51754 HCl; Lot# 0505031-15