4-Methyldiethcathinone (4-MDEC)

Sample Type: Seized Material

Latest Revision: May 18th, 2018
Date Received: December 12th, 2017
Date of Report: February 27th, 2018

1. GENERAL INFORMATION

IUPAC Name: 2-(diethylamino)-1-(4-methylphenyl)propan-1-one
InChI String: InChI=1S/C14H21NO/c1-5-15(6-2)12(4)14(16)13-9-7-11(3)8-10-13/h7-10,12H,5-6H2,1-4H3
CFR: Not Scheduled (02/2018)
CAS# 676316-90-8
Synonyms: N,N-diethyl-4-methylcathinone; N,N-DEMC; 4-MEC ET, MDEC
Source: Department of Homeland Security
Appearance: Off-white solid material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M+]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₄H₂₁NO</td>
<td>219.3</td>
<td>219</td>
<td>220.1696</td>
</tr>
</tbody>
</table>

*Important Note*: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

*Prepared By*: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT
3. BRIEF DESCRIPTION

4-Methyldiethcathinone is classified as a substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Substituted cathinones have been reported to cause stimulant-like effects, similar to amphetamines, which are structurally related to substituted cathinones. Substituted cathinones have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include cathinone, mephedrone (4-methylmethcathinone), 4-methylethcathinone (4-MEC), ethcathinone (ETH-CAT), and N,N-diethylethcathinone. Cathinone, mephedrone, and 4-MEC are all explicitly Schedule I substances in the United States, while ethcathinone is listed as a mephedrone isomer.

4. ADDITIONAL RESOURCES

https://www.chemspider.com/Chemical-Structure.28593991.html

https://comptox.epa.gov/dashboard/dsstoxdb/results?exact=1&mass=0&search=655742&single_component=0

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-MDEC-ID-1858-17_report.pdf

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)
Sample Preparation: Acid/Base extraction
Instrument: Agilent 5975 Series GC/MSD System
Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas: Helium (Flow: 1 mL/min)
Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C
Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:**
- Injection Type: Splitless
- Injection Volume: 1 µL

**MS Parameters:**
- Mass Scan Range: 40-550 m/z
- Threshold: 250

**Retention Time:**
4.323 min

**GC Chromatogram: 4-Methyldiethcathinone (4-MDEC)**

Additional peaks present in chromatogram: internal standard 1 (3.134 min), probable breakdown (4.597 min), internal standard 2 (6.200 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-Methyldiethcathinone (4-MDEC)
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: 1:10 dilution of acid/base extraction in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase: A: Ammonium formate (10 mM, pH 3.0)

B: Methanol/acetonitrile (50:50)

Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures: Autosampler: 15 °C

Column Oven: 30 °C

Source Heater: 600 °C

Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 4.94 min
LC Chromatogram: 4-Methyldiethcathinone (4-MDEC)

TOF MS (Top) and MS/MS (Bottom) Spectra: 4-Methyldiethcathinone (4-MDEC)
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in CDCl₃

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters:
- Pulse Sequence: Proton
- Solvent: CDCl₃
- Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D
- Delay between pulses: 1st delay, d1 = 1.000
$^1$H NMR: 4-Methylidethcathinone (4-MDEC)

$^1$H NMR (300 MHz, CHLOROFORM-d) δ ppm 8.01 (d, J=8.20 Hz, 2 H) 7.20 - 7.26 (m, 4 H) 4.36 (s, 1 H) 4.33 (s, 1 H) 2.64 (s, 1 H) 2.53 - 2.63 (m, 3 H) 2.40 (s, 3 H) 2.27 (d, J=6.44 Hz, 3 H) 0.98 - 1.04 (m, 6 H) 0.60 (s, 1 H)

gCOSY: 4-Methylidethcathinone (4-MDEC)
### 6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
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<tbody>
<tr>
<td>05/18/2018</td>
<td>Added “Sample Type: Seized Material” to Page 1.</td>
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<td>Added “Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT” to Page 1 footer.</td>
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