**N-Cyclohexyl Methylone**

Sample Type: **Drug Material**

Latest Revision: **May 9, 2022**

Date Received: **January 25, 2022**

Date of Report: **May 9, 2022**

1. **GENERAL INFORMATION**

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(cyclohexylamino)propan-1-one

**InChI String:** InChI=1S/C16H21NO3/c1-11(17-13-5-3-2-4-6-13)16(18)12-7-8-14-15(9-12)20-10-19-14/h7-9,11,13,17H,2-6,10H2,1H3

**CFR:** Not Scheduled (05/2022)

**CAS#** Not Available

**Synonyms:** Cyputylone, 3,4-Methylenedioxy-N-Cyclohexylcathinone, 3,4-Methylenedioxy-α-Cyclohexylaminopropiophenone

**Source:**
- (1) Indianapolis-Marion County Forensic Services Agency
- (2) Miami Dade Police Department

**Appearance:**
- (1) Ecstasy Tablet
- (2) Beige Crystalline Rock and Off-White Crystalline Powder

**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.

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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>C₁₆H₂₁NO₃</td>
<td>275.3</td>
<td>275</td>
<td>276.1594</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

*N*-Cyclohexyl methylone is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause psychoactive effects similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar drugs include methylone and diethlyone (or *N,N-*diethyl methylone), among other *beta*-keto methylenedioxyamphetamine (or “*-ylones”). Methylone is a Schedule I substance in the United States; *N*-cyclohexyl methylone is not explicitly scheduled.

*N*-Cyclohexyl methylone has been mentioned in online drug forums and appeared for sale on surface web gray market vendor sites under the name “cyputylone”. Scientific experts agree that the name “cyputylone” is not preferred due to nomenclature inconsistency and potential for confusion, and rather suggest the name “*N*-cyclohexyl methylone” be universally used instead.

4. ADDITIONAL RESOURCES

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

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

Sample Preparation: Dilution in methanol (Miami Dade Police Department)

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures:
- Injection Port: 265 °C
- Transfer Line: 300 °C
- MS Source: 230 °C
- MS Quad: 150 °C
- Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

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

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

Retention Time: 6.22 min

Standard Comparison: Reference material for N-Cyclohexyl Methylone (Batch: 0628328-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-Cyclohexyl Methylone based on retention time (6.20 min) and mass spectral data. (https://www.caymanchem.com/product/35165/3%2C4-methylenedioxy-%CE%B1-cyclohexylaminopropiophenone-(hydrochloride))
Chromatogram: $N$-Cyclohexyl Methylone

Additional peaks in chromatogram: internal standards (3.06 and 5.70 mins)

EI (70 eV) Mass Spectrum: $N$-Cyclohexyl Methylone
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: Dilution in methanol (Miami Dade Police Department) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)

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: 5.93 min

Standard Comparison: Reference material for N-Cyclohexyl Methylone (Batch: 0628328-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-Cyclohexyl Methylone based on retention time (5.84 min) and mass spectral data. (https://www.caymanchem.com/product/35165/3%2C4-methylenedioxy-%CE%B1-cyclohexylaminopropiophenone-(hydrochloride))
Extracted Ion Chromatogram: \textit{N}-Cyclohexyl Methylone

TOF MS Spectra: \textit{N}-Cyclohexyl Methylone
6. FUNDING

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