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
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>C₁₉H₂₆FN₃O₃</td>
<td>363.4</td>
<td>363</td>
<td>364.2031</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

4F-MDMB-BINACA is classified as a synthetic cannabinoid. Synthetic cannabinoids have been reported to cause psychoactive effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. 5F-MDMB-PINACA (5F-ADB) is a structurally similar compound and Schedule I substance in the United States.

4. ADDITIONAL RESOURCES


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:** 7.443 min

**Chromatogram:** 4F-MDMB-BINACA

*Additional peaks present in chromatogram: internal standard 1 (3.210 min) and internal standard 2 (6.281 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-MDMB-BINACA
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: 1:100 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 ºC

Column Oven: 30 ºC

Source Heater: 600 ºC

Injection Parameters: Injection Volume: 10 µL

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

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 9.16 min
Chromatogram: 4F-MDMB-BINACA
TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-MDMB-BINACA
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

¹H NMR: 4F-MDMB-BINACA