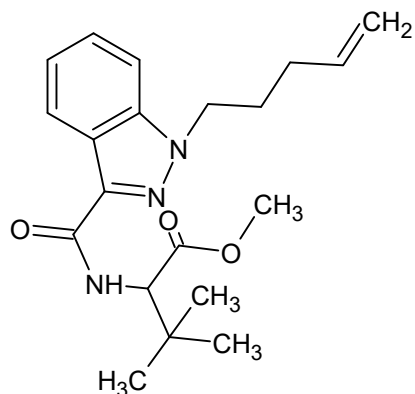




## MDMB-4en-PINACA

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	Methyl 3,3-dimethyl-2-(1-(pent-4-en-1-yl)-1H-indazole-3-carboxamido)butanoate
<b>CAS#:</b>	2504100-70-1
<b>Synonyms:</b>	MDMB-PENINACA, Methyl 3-methyl-N-[1-(pent-4-en-1-yl)-1H-indazole-3-carbonyl]valinate, Methyl 3-methyl-N- {[1-(pent-4-en-1-yl)-1H-indazole-3-yl]carbonyl} valinate
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>UV<sub>max</sub>(nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>	357.45	54.19



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## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~11 mg/mL in CD<sub>3</sub>OD containing TMS for 0 ppm reference and 1,4-BTMSB-d<sub>4</sub> as quantitative internal standard.

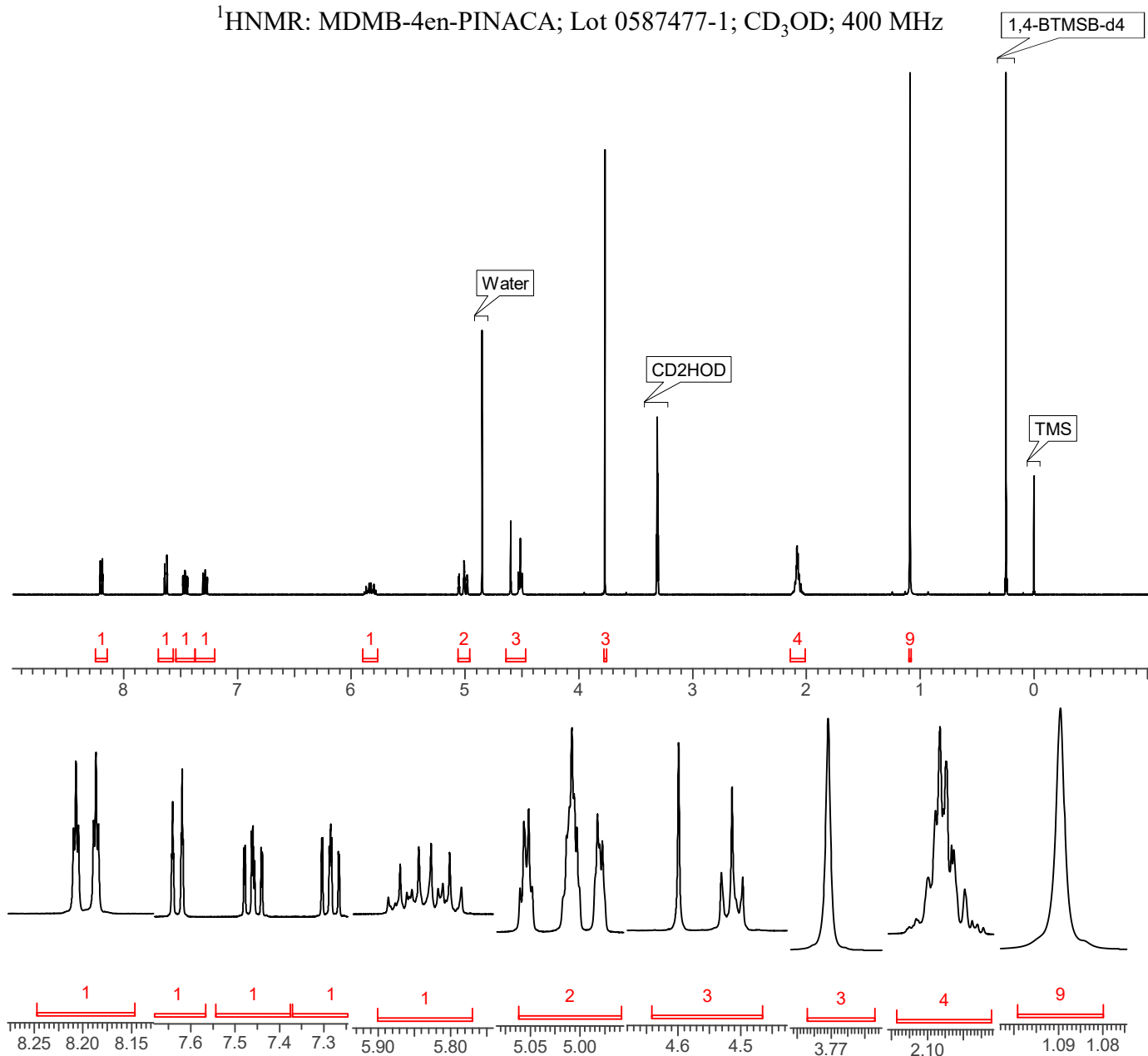
**Instrument:** 400 MHz NMR spectrometer

**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>HNMR: MDMB-4en-PINACA; Lot 0587477-1; CD<sub>3</sub>OD; 400 MHz





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## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

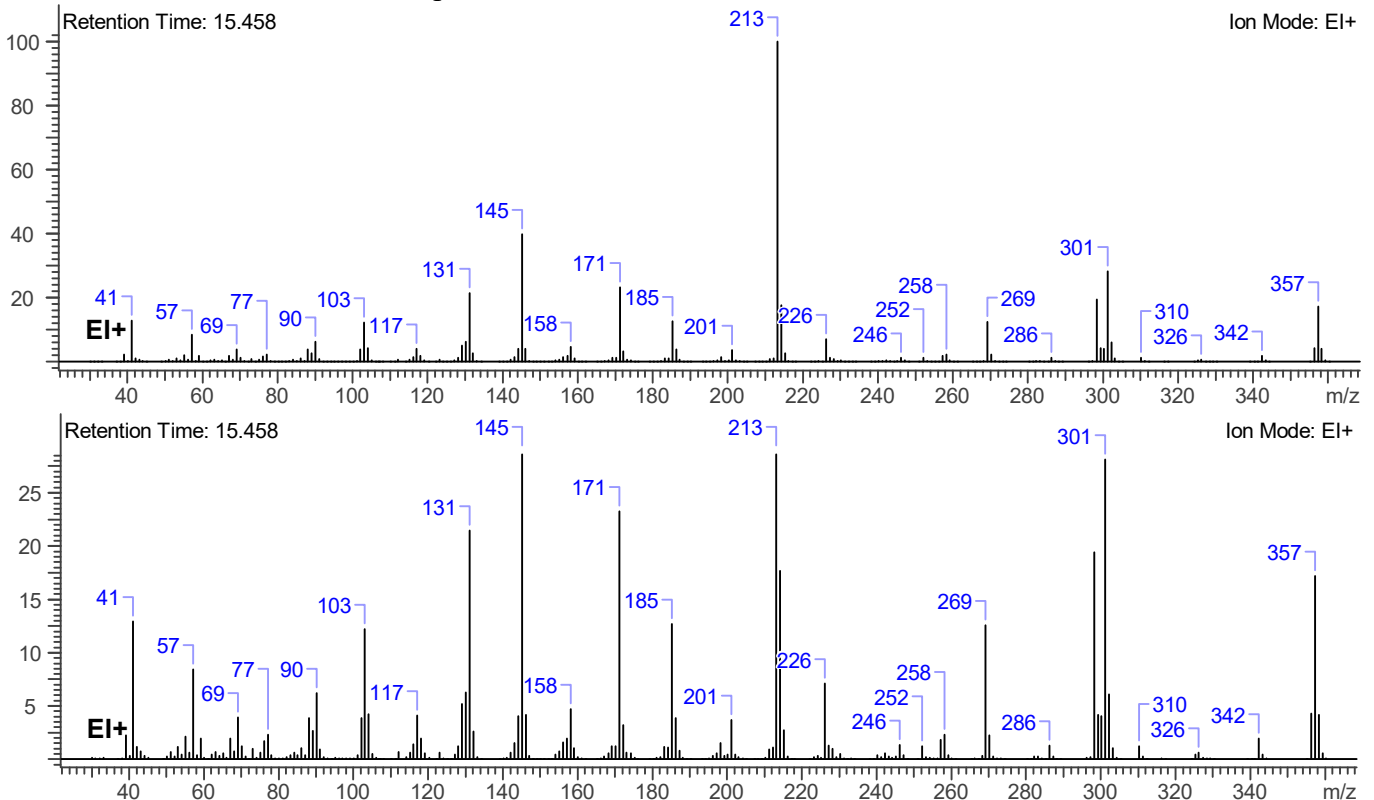
**Sample Preparation:** Dilute analyte ~4mg/mL in CH<sub>3</sub>OH.

**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:** 15.456 min

EI Mass Spectrum: MDMB-4en-PINACA; Lot #0587477-1





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## 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<sup>-1</sup>  
Sample gain: 1  
Aperture: 150

FTIR ATR (Diamond 1 Bounce): MDMB-4en-PINACA; Lot# 0587477-1

