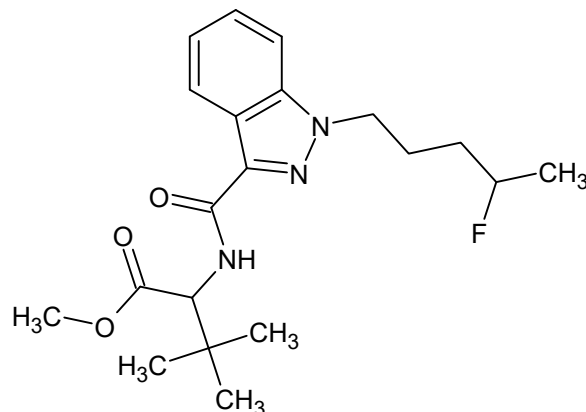




## 4-Fluoro ADB

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



### 1. GENERAL INFORMATION

**IUPAC Name:** methyl 2-(1-(4-fluoropentyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate

**CAS#:** NA

**Synonyms:** 4-Fluoro-MDMB-PINACA; methyl 2- {[1-(4-fluoropentyl)-1H-indazole-3-carbonyl]amino}-3,3-dimethylbutanoate

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV<sub>max</sub>(nm):** 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>28</sub> FN <sub>3</sub> O <sub>3</sub>	377.45	47.26



## 4-Fluoro ADB

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



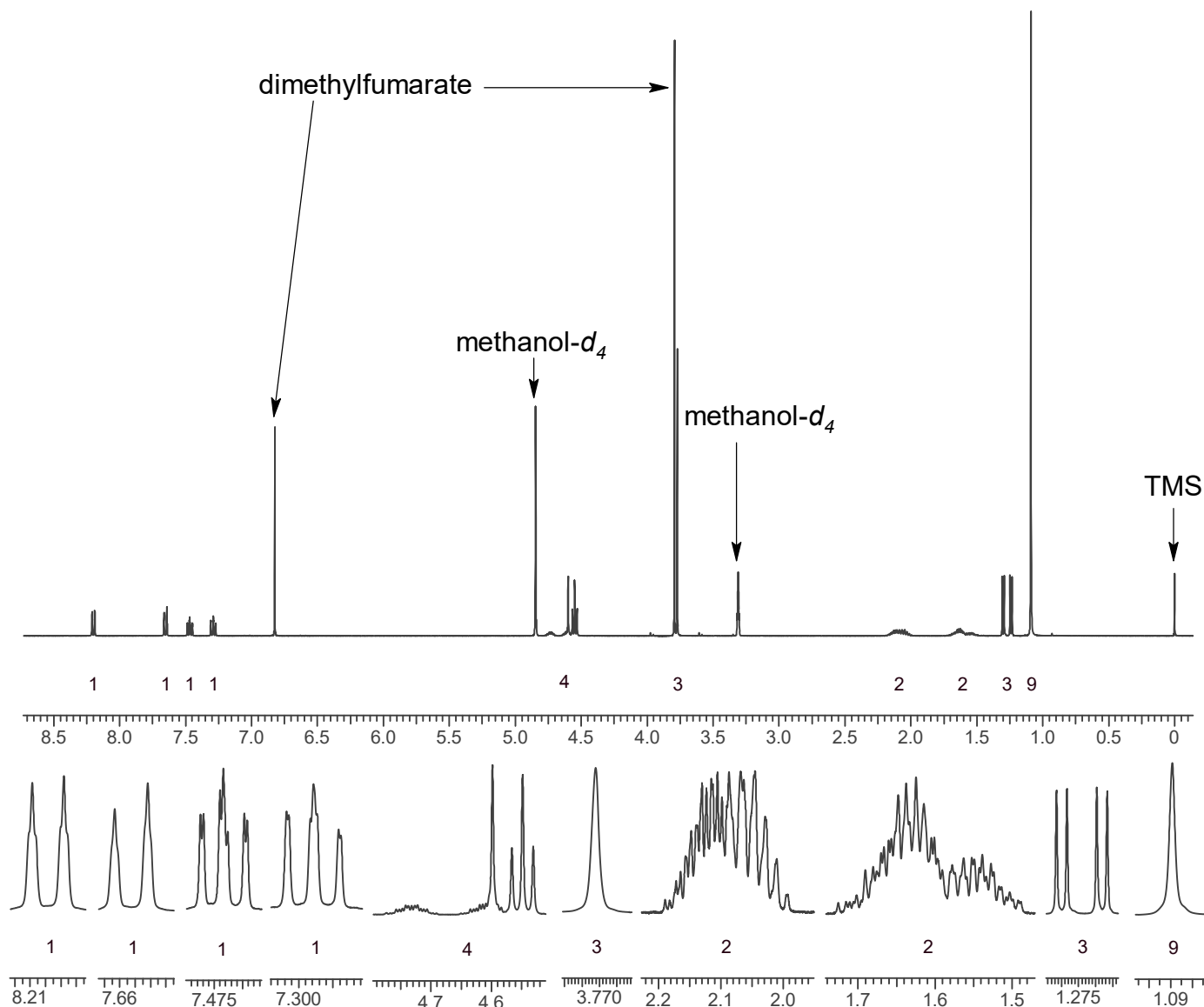
### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~11 mg/mL in methanol- $d_4$  containing TMS for 0 ppm reference and dimethylfumarate 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

$^1\text{H}$ NMR: 4-Fluoro ADB; Lot # 0524165-1;  $\text{CD}_3\text{OD}$ ; 400MHz





## 4-Fluoro ADB

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

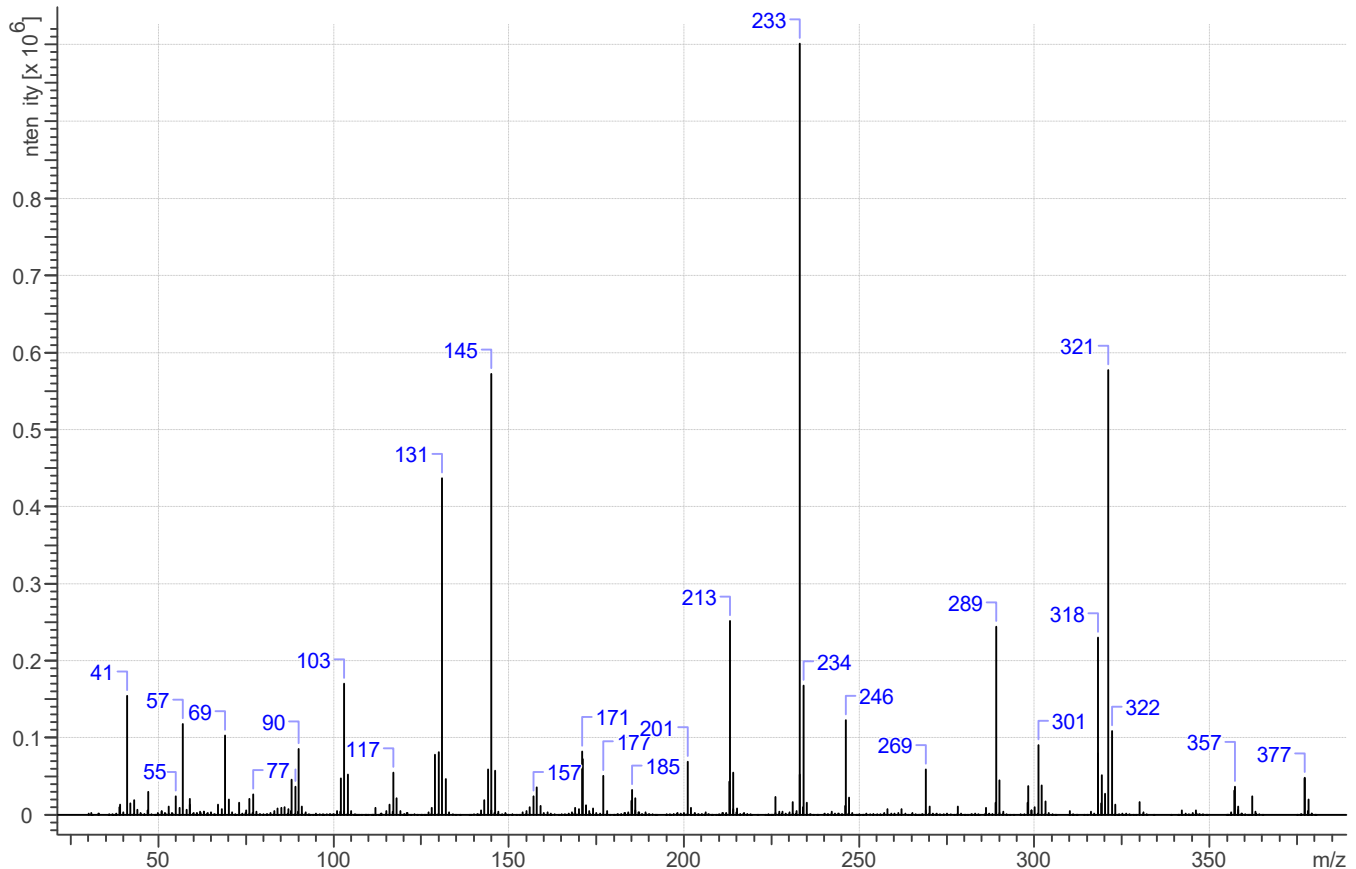


### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**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: 250  
Tune file: stune.u                      Acquisitionmode: scan  
**Retention Time:** 16.044 min

EI Mass Spectrum: 4-Fluoro ADB; Lot # 0524165-1





# 4-Fluoro ADB

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



## 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): 4-Fluoro ADB; Lot # 0524165-1

