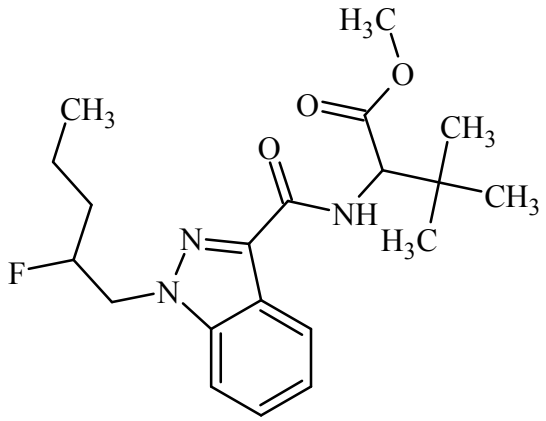
2-Fluoro-ADB

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-(2-fluoropetnyl)-1*H*-indazole-3-carboxamido -3,3-dimethylbutanoate

CAS#: N/A

Synonyms: 2-Fluoro-MDMB-PINACA

Source: DEA Reference Material Collection

Appearance: White Powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

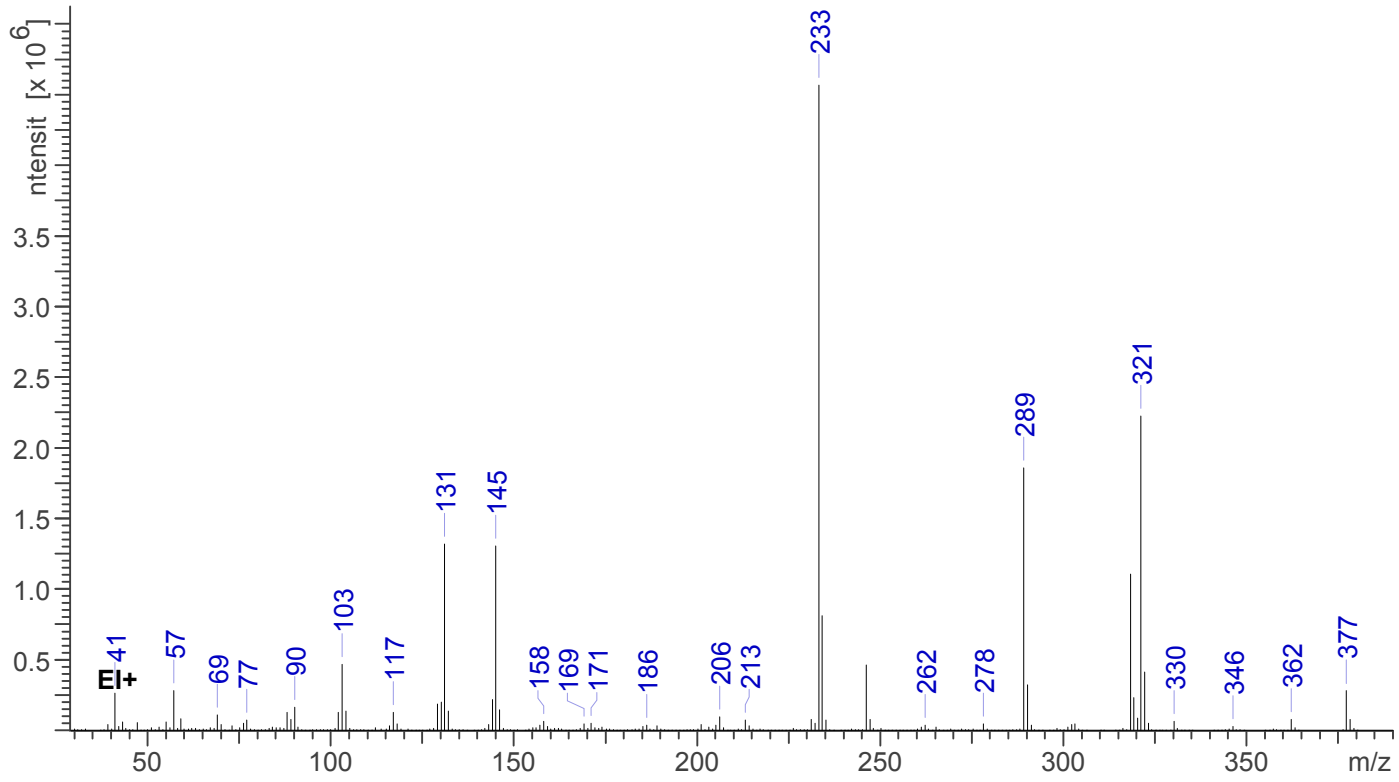
Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{20}H_{28}FN_3O_3$	377.45	Not Determined

3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in chloroform.

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 30.0 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:	15.743 min

EI Mass Spectrum: 2-Fluoro-ADB; Lot 0481551-2



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^{-1}
Sample gain: 1
Aperture: 150

FTIR (Diamond ATR, 1 Bounce): 2-Fluoro-ADB; Lot 0481551-2