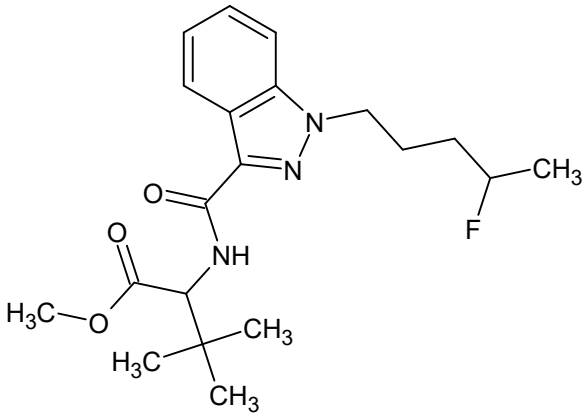
4-Fluoro ADB

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



1. GENERAL INFORMATION

IUPAC Name: methyl *N*-[1-(4-fluoropentyl)-1*H*-indazole-3-carbonyl]-3-methylvalinate

CAS#: NA

Synonyms: 4-Fluoro-MDMB-PINACA; methyl 2-(1-(4-fluoropentyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate

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	47.26

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11.5 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}HNMR: 4-Fluoro ADB; Lot # 0524165-1; CD_3OD; 400MHz