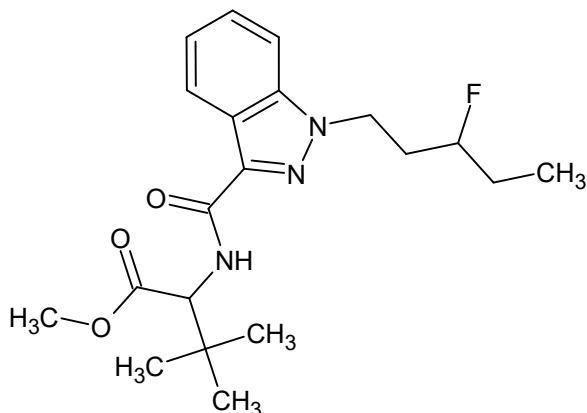




3-Fluoro ADB

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-(3-fluoropentyl)-1*H*-indazole-3-carbonyl]-3-methylvalinate

CAS#: NA

Synonyms: 3-Fluoro-MDMB-PINACA; methyl 2-(1-(3-fluoropentyl)-1*H*-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 (°C)
Base	C ₂₀ H ₂₈ FN ₃ O ₃	377.45	Not Determined



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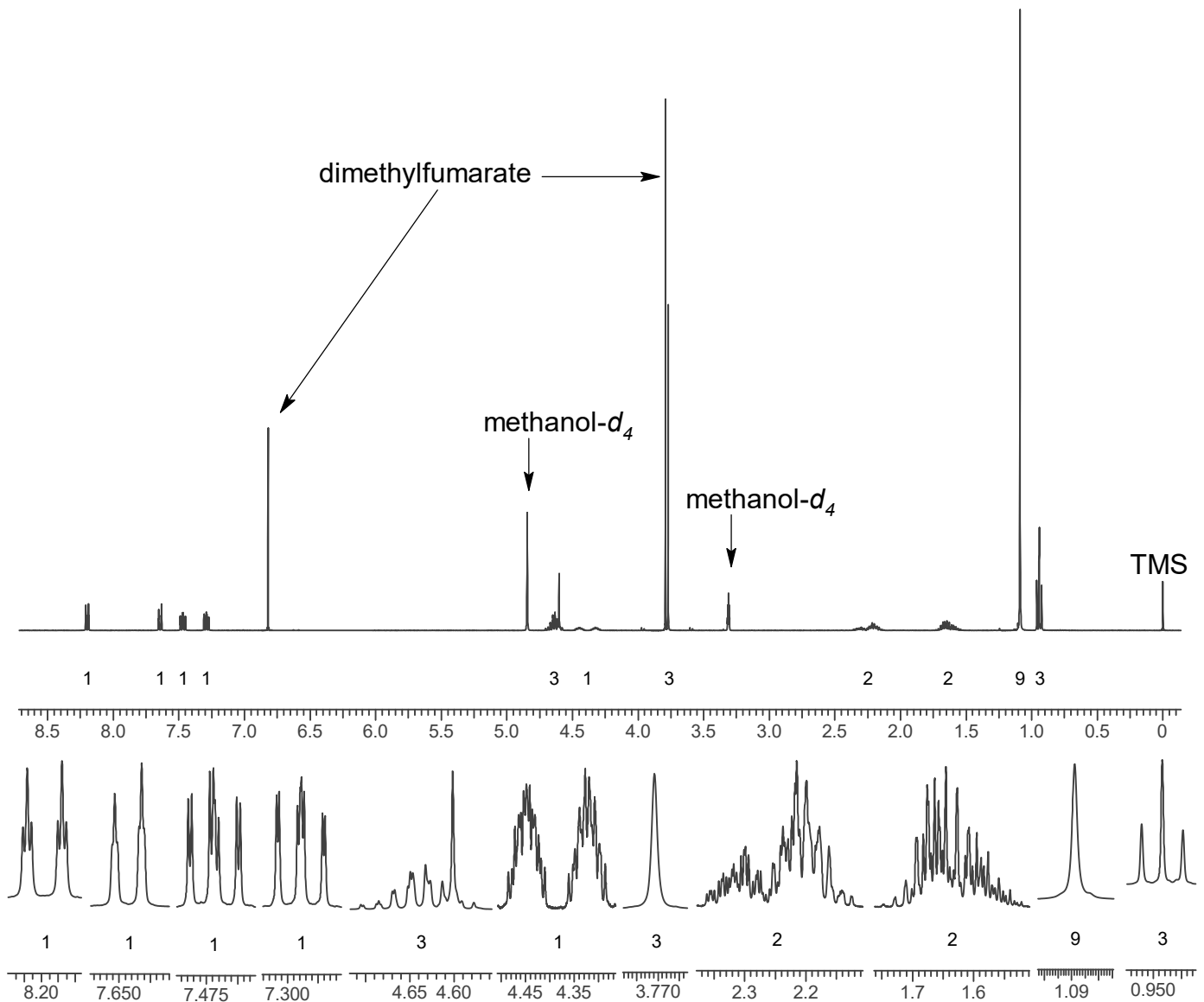
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~19.2 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

^1H NMR: 3-Fluoro ADB; Lot # 0481552-2; CD_3OD ; 400MHz





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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⁻¹
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 3-Fluoro ADB; Lot # 0481552-2

