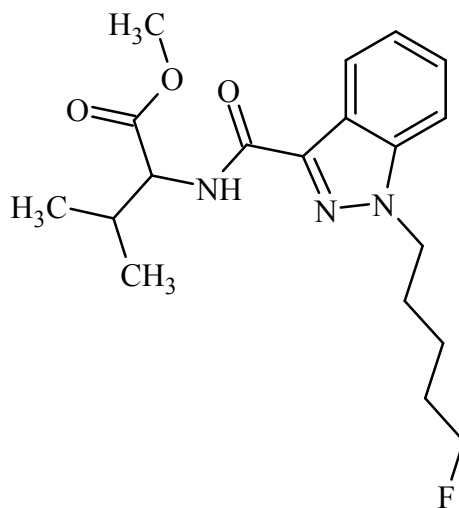




5-Fluoro-AMB

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-(5-fluoropentyl)-1*H*-indazol-3-yl]carbonyl} valinate
- CAS#:** Not Available
- Synonyms:** 5-Fluoro-AMP, (S)-methyl 2-(1-(5-fluoropentyl)-1*H*-indazole-3-carboxamido)-3-methylbutanoate
- 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 ₁₉ H ₂₆ FN ₃ O ₃	363	70.9-72.6



5-Fluoro-AMB

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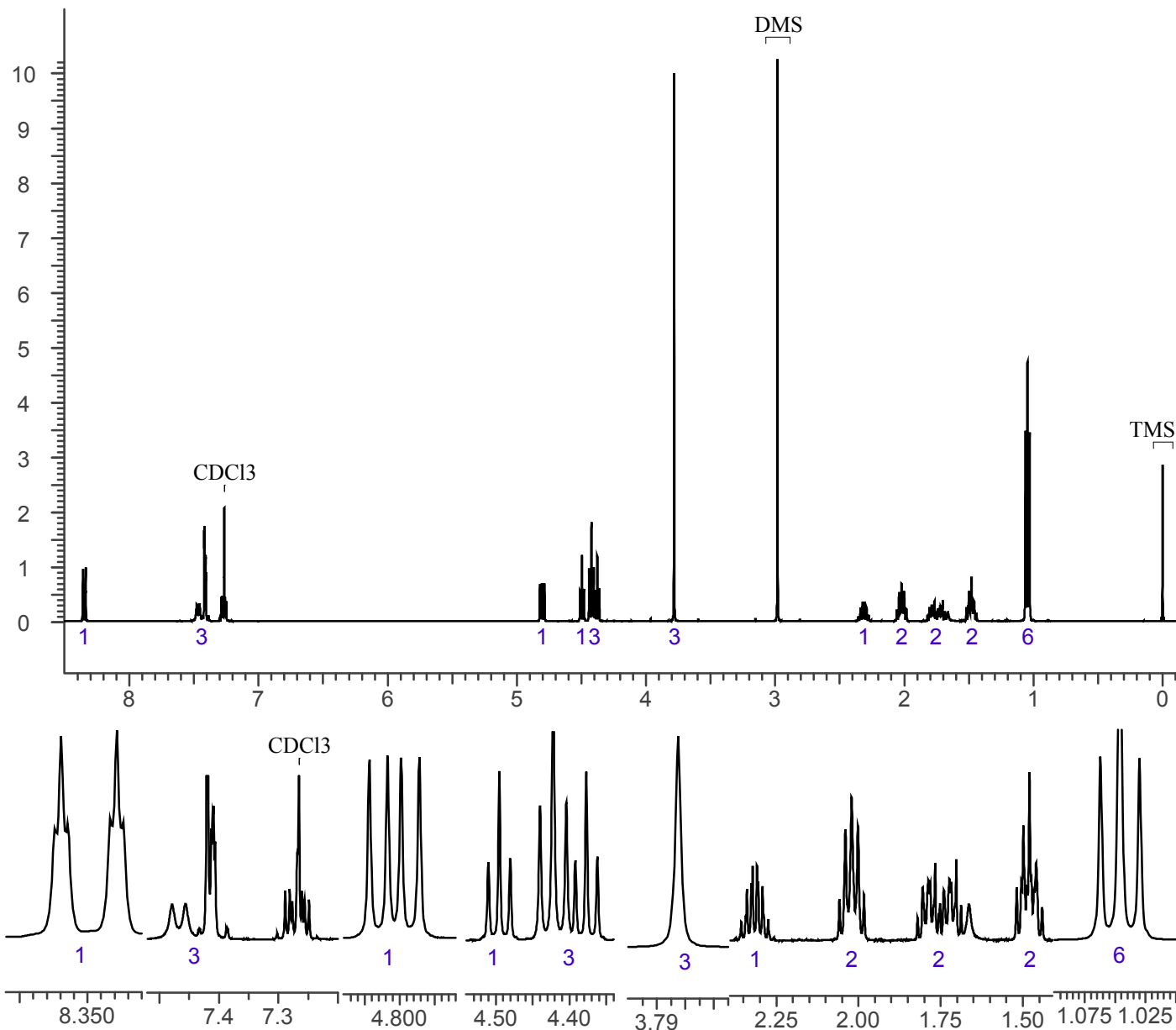


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylsulfone 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 5-Fluoro-AMB Lot RM-140318-04, CDCl₃, 400MHz





5-Fluoro-AMB

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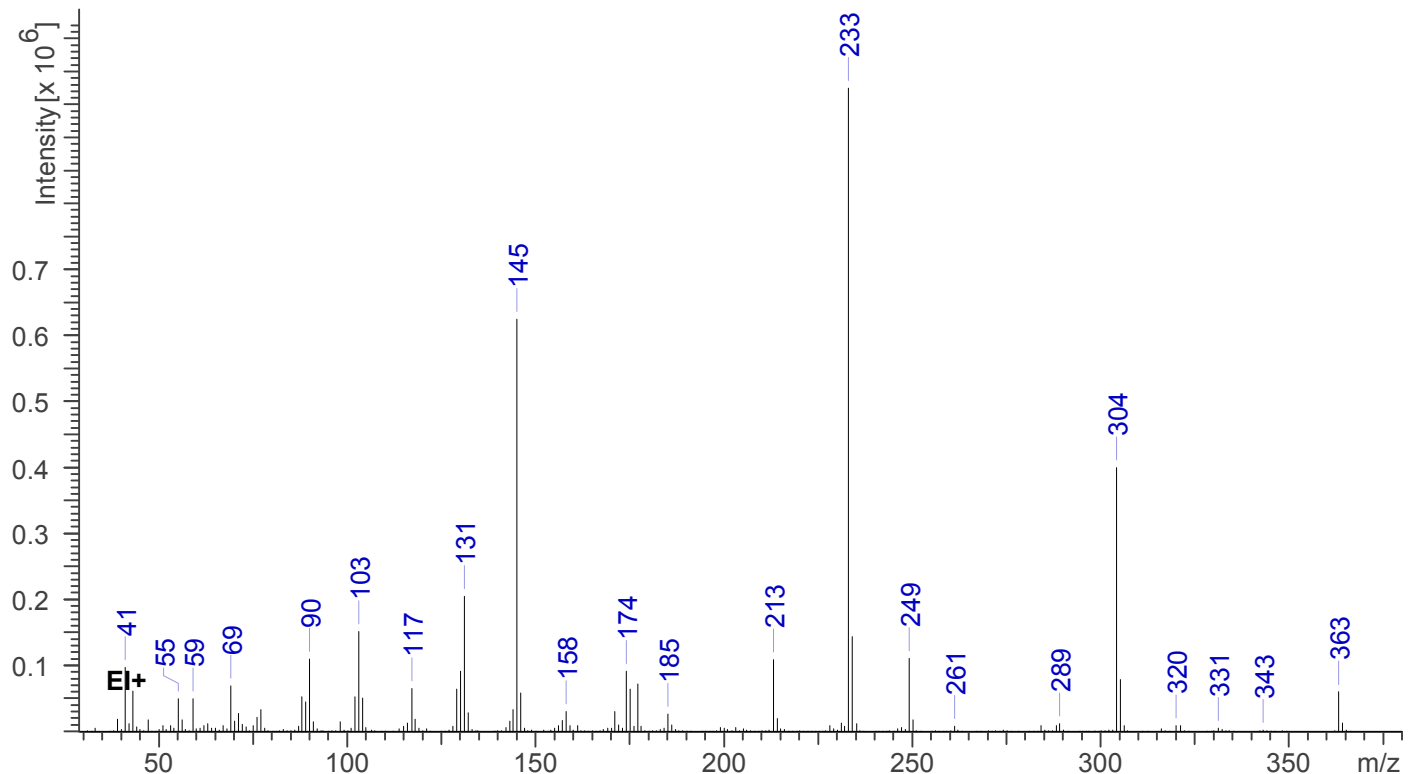
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1 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 300°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 15.614 min

EI Spectrum, 5-Fluoro-AMB Lot RM-140318-04





5-Fluoro-AMB

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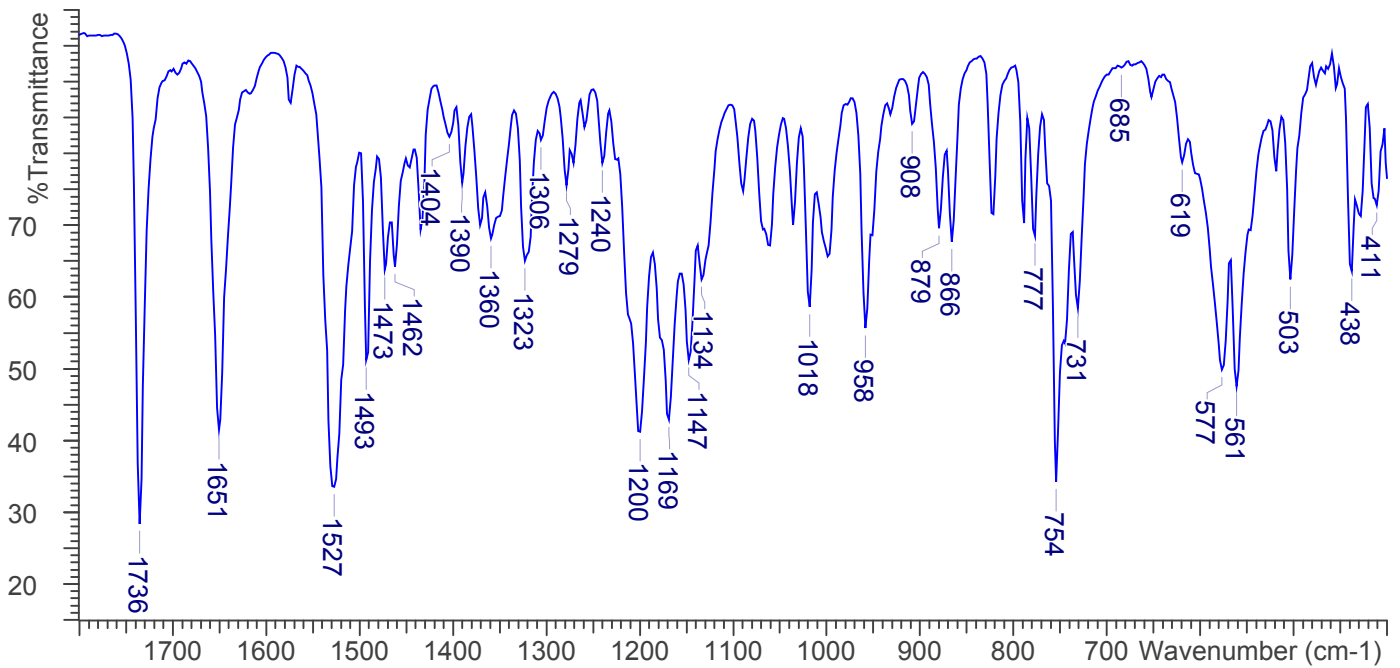
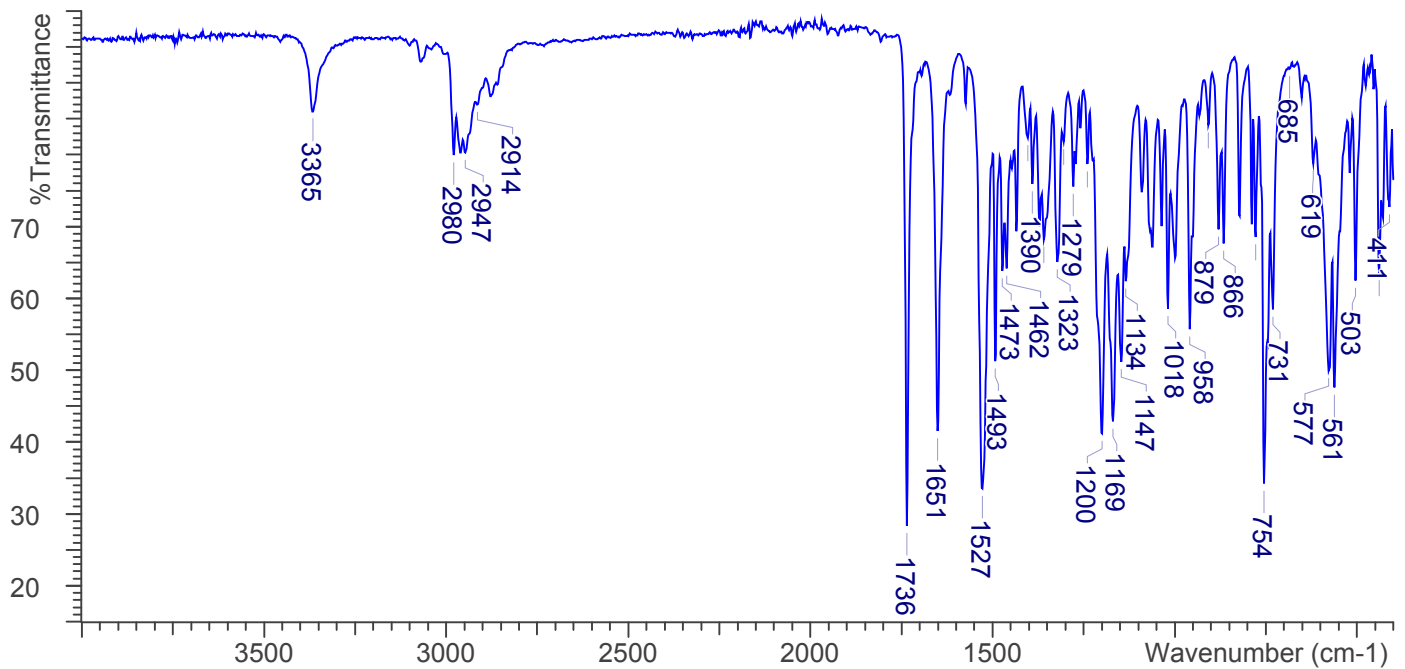


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond 3-Bounce) 5-Fluoro-AMB Lot RM-140318-04





5-Fluoro-AMB

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4. ADDITIONAL RESOURCES

No Literature Available as of 08/2014.