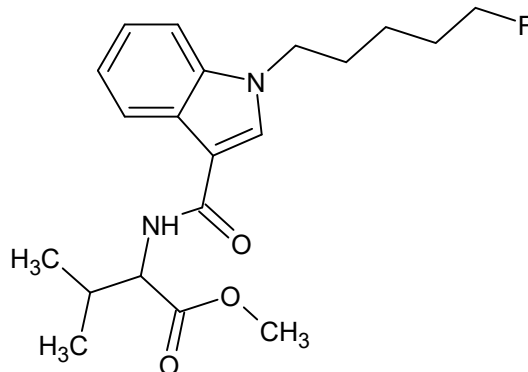




MMB-2201

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



1. GENERAL INFORMATION

| | |
|------------------------------|---|
| IUPACName: | methyl <i>N</i> -[1-(5-fluoropentyl)-1 <i>H</i> -indole-3-carbonyl]valinate |
| CAS#: | 1616253-26-9 |
| Synonyms: | AMB-PICA, I-AMB, methyl 2-(1-(5-fluoropentyl)-1 <i>H</i> -indole-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 ₂₀ H ₂₇ FN ₂ O ₃ | 362.44 | Not Determined |



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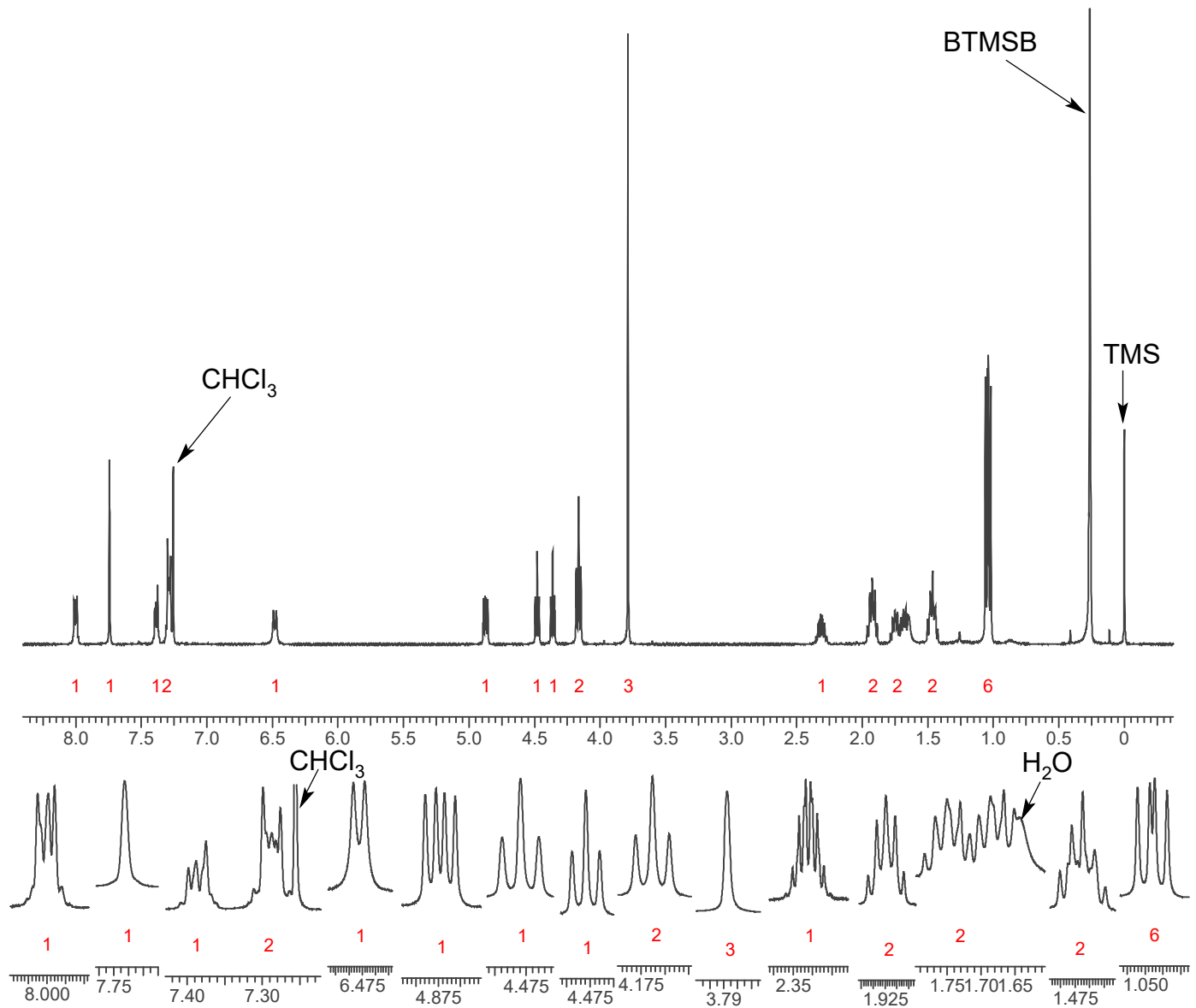
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~7 mg/mL in CDCl_3 containing TMS for 0 ppm reference and BTMSB 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: MMB-2201; Lot # 0457890-18; CDCl_3 ; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

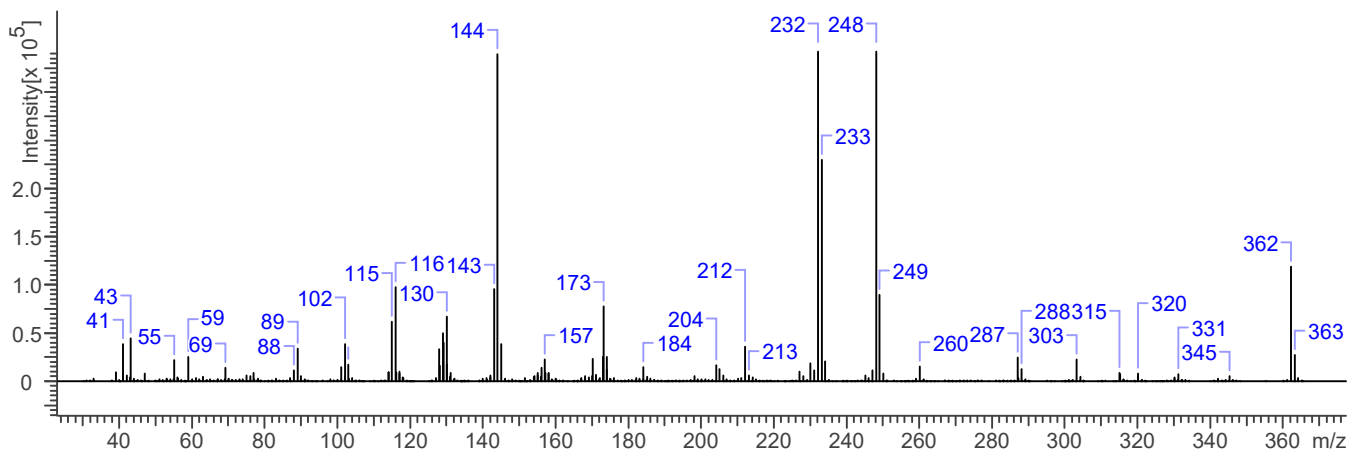
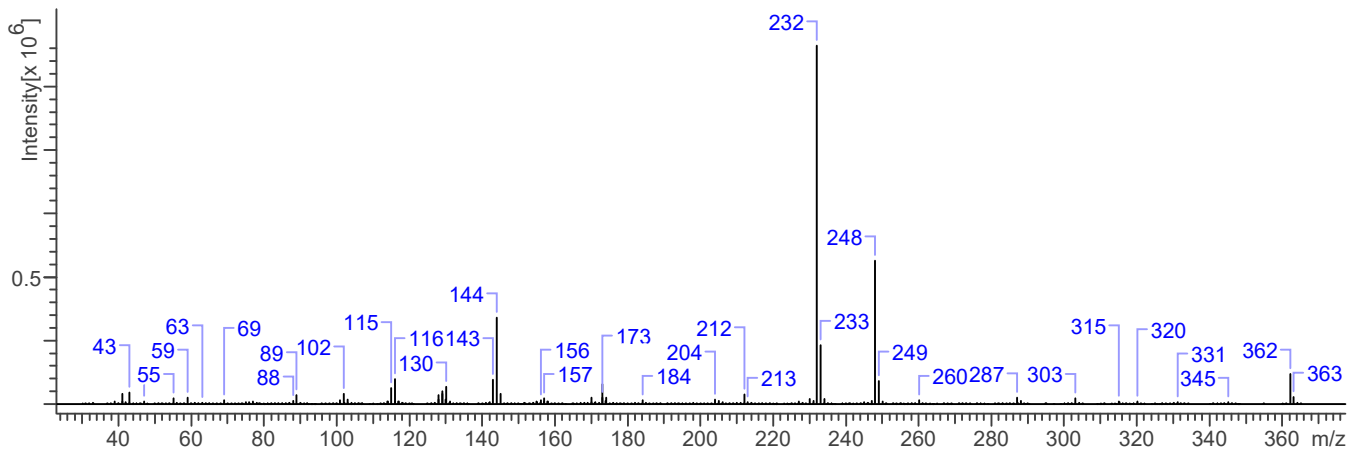
Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5 mL/min
Temperatures: Injector: 280°C MSD transfer line: 280°C
MS Source: 230°C MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 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 Acquisition mode: scan

Retention Time: 18.136 min

EI Mass Spectrum: MMB-2201; Lot # 0457890-18





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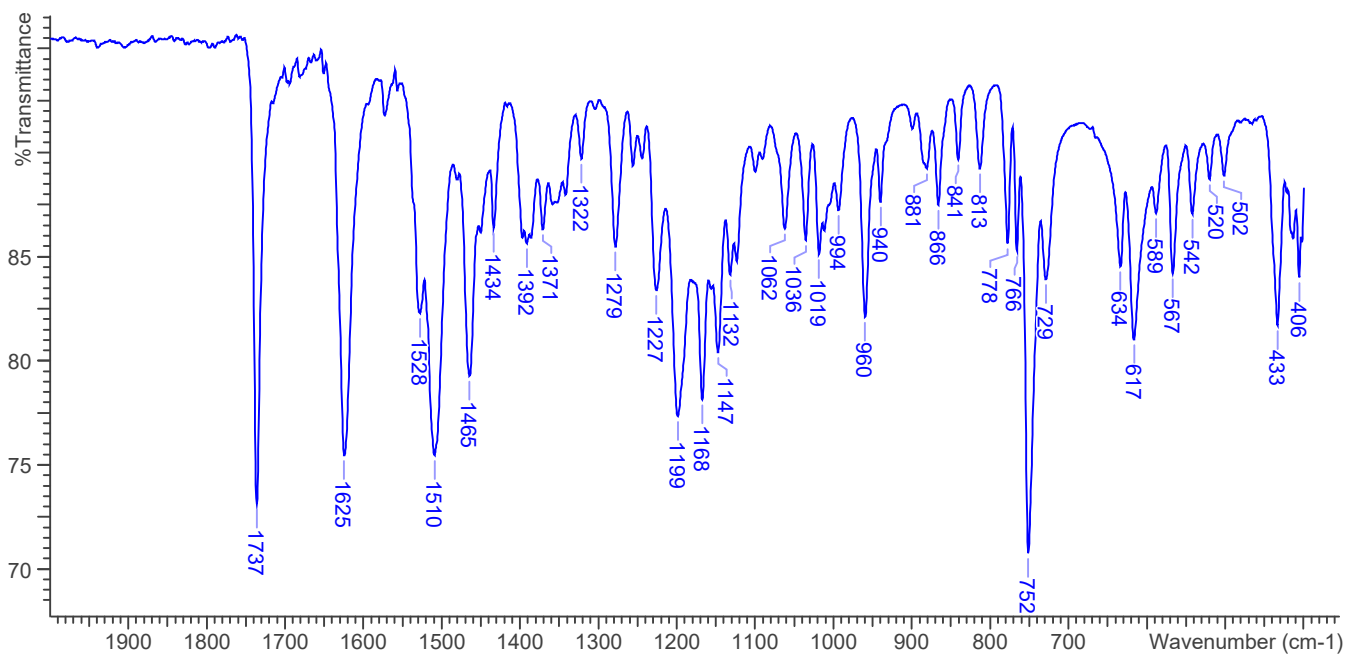
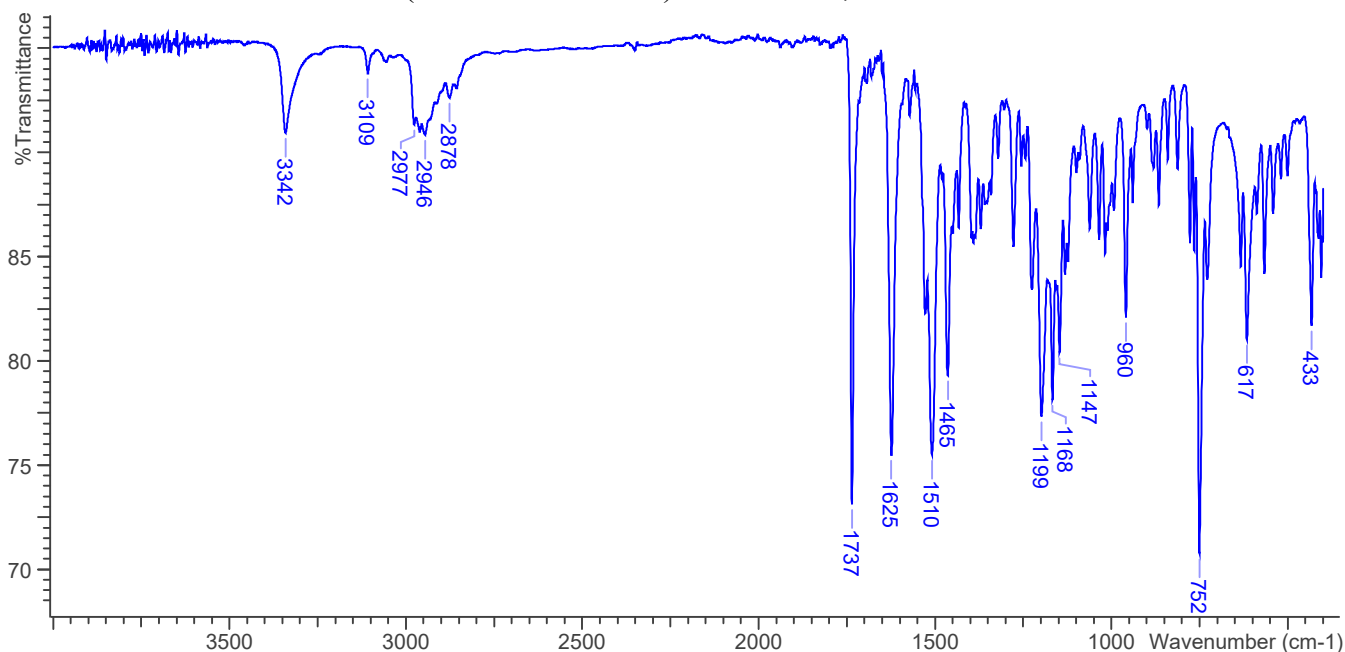


3.3 INFRARED SPECTROSCOPY (FTIR)

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): MMB-2201; Lot # 0457890-18





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4. ADDITIONAL RESOURCES

[Wikipedia](#)