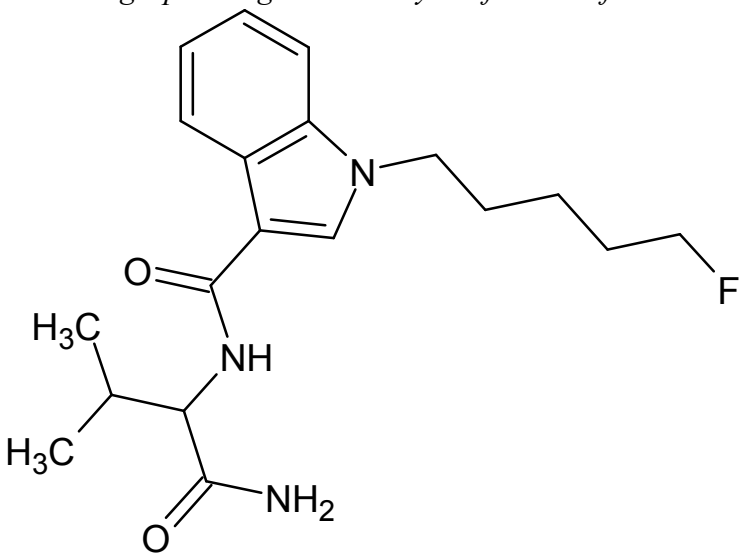
5-Fluoro-ABICA

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



1. GENERAL INFORMATION

IUPAC Name: *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl-1*H*-indole-3-carboxamide

CAS#: Not Available

Synonyms: 5F-ABICA

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	$C_{19}H_{26}FN_3O_2$	347	201.1

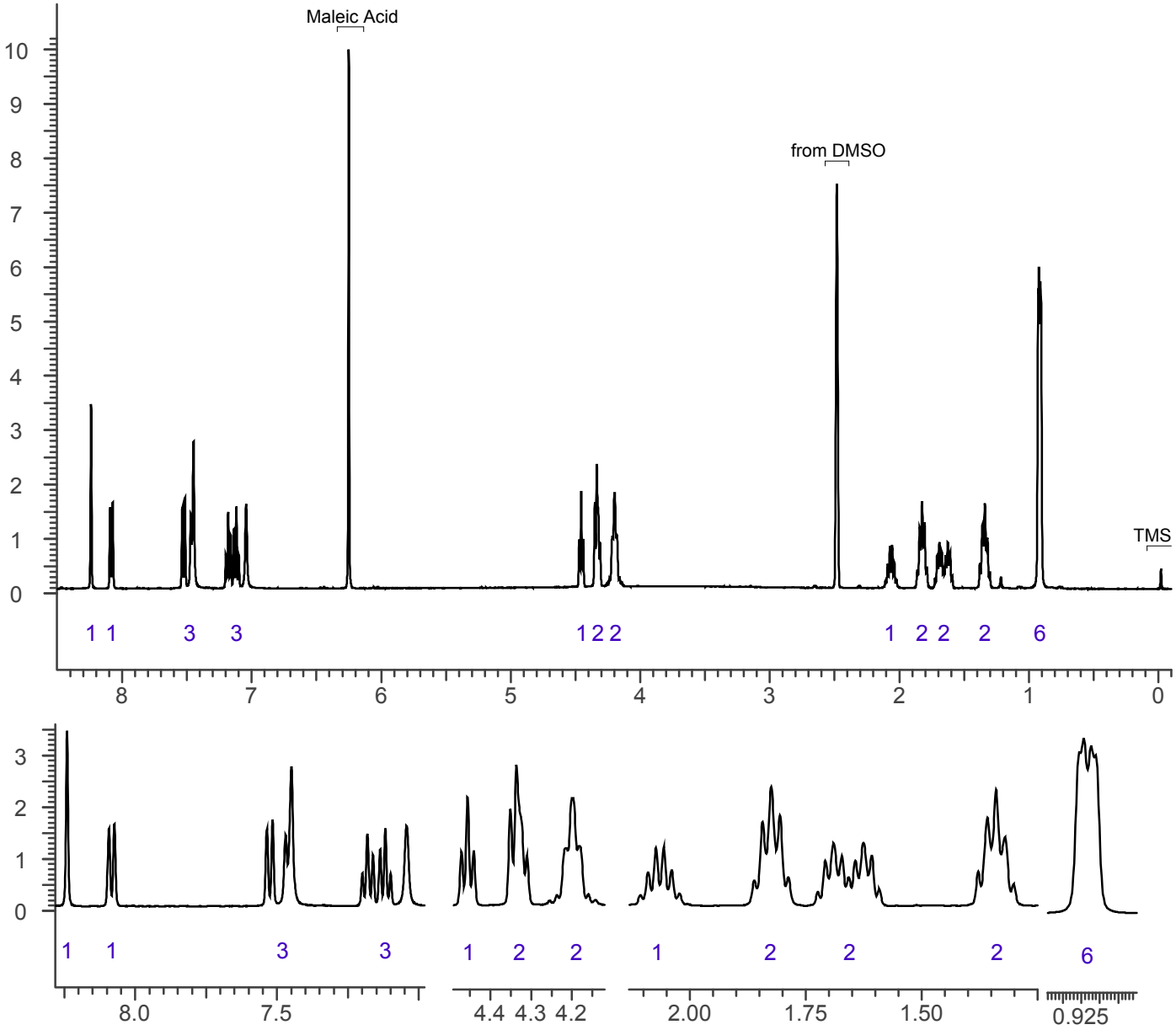
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in DMSO containing TMS for 0 ppm reference and maleic acid 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}H NMR: 5-fluoro-ABICA Lot # 0456711-14; DMSO; 400MHz

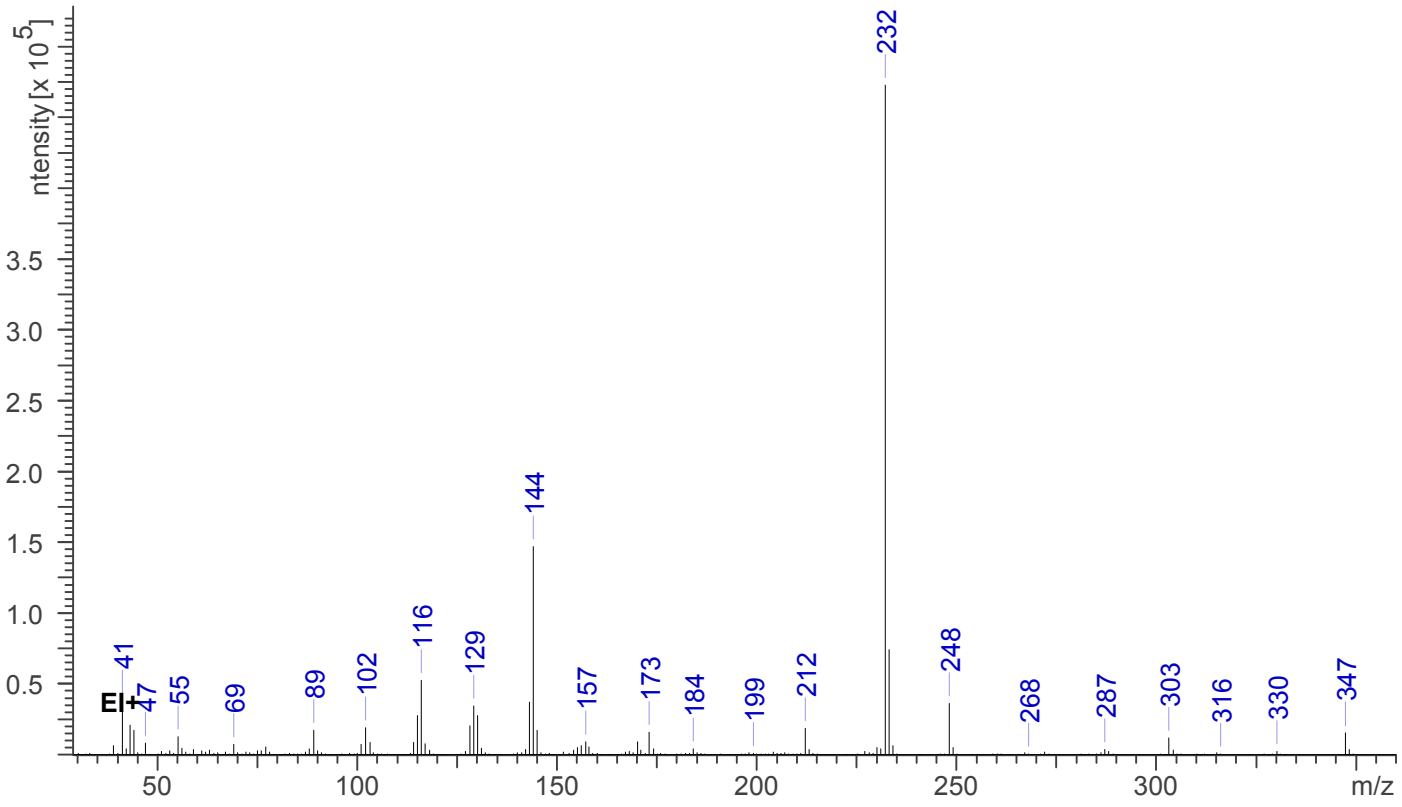


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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 25.0 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:	18.030 min

EI Mass Spectrum: 5-fluoro-ABICA Lot # 0456711-14

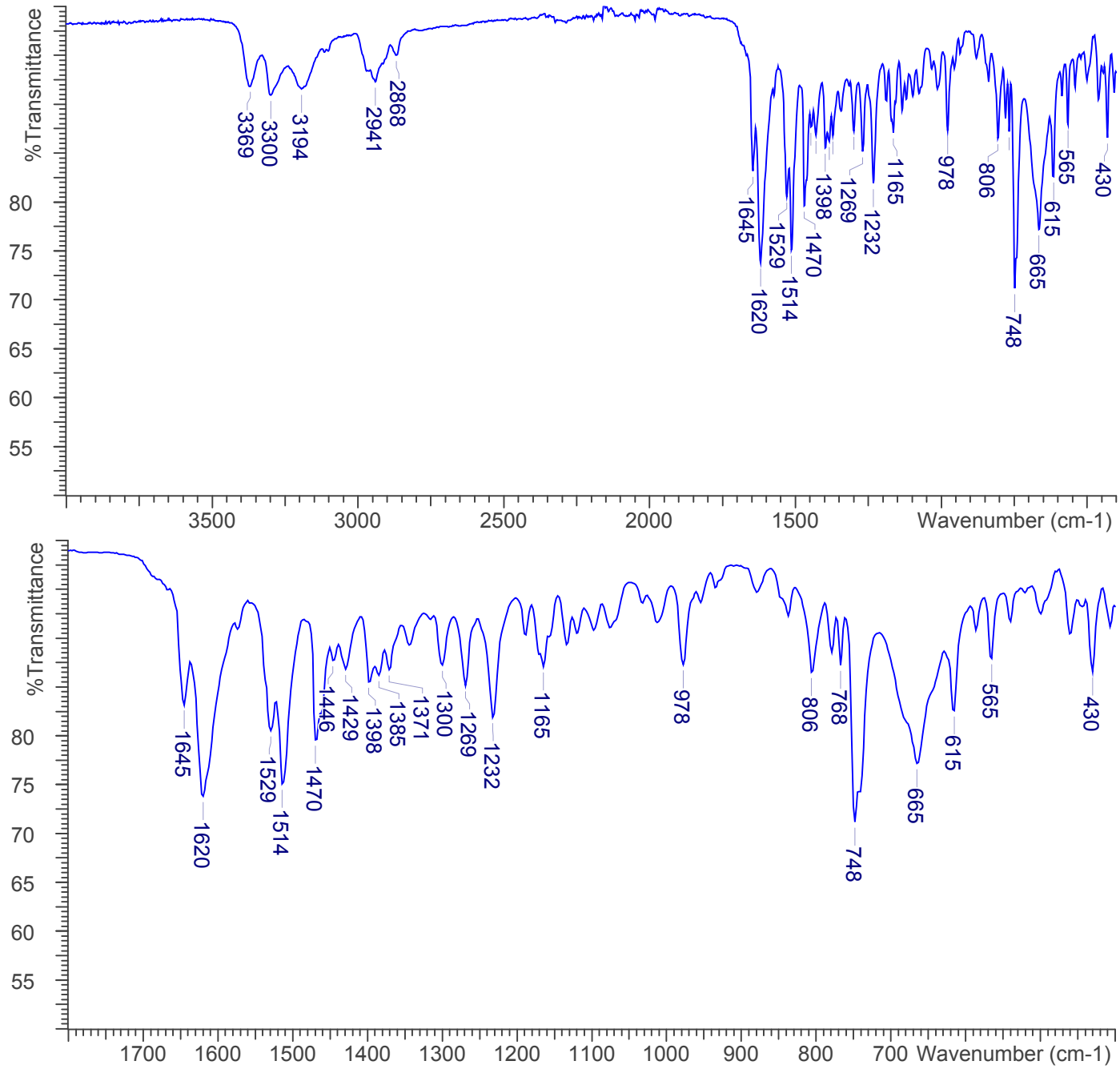


3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: 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-ABICA Lot # 0456711-14



4. ADDITIONAL RESOURCES

No resources identified as of 12/01/14.