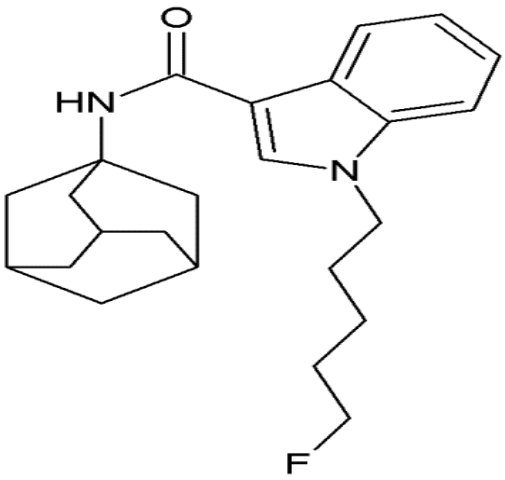
STS-135

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



1. GENERAL INFORMATION

IUPAC Name:	1-(5-fluoropentyl)-N-(tricyclo[3.3.1.1^{3,7}]dec-1-yl)-1*H*-indole-3-carboxamide
CAS #:	1354631-26-7
Synonyms:	N-adamantyl-1-fluoropentylindole-3-carboxamide, 5F-2NE1
Source:	DEA Reference Material Collection
Appearance:	White powder
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{24}H_{31}FN_2O$	382	138.6

3. QUALITATIVE DATA

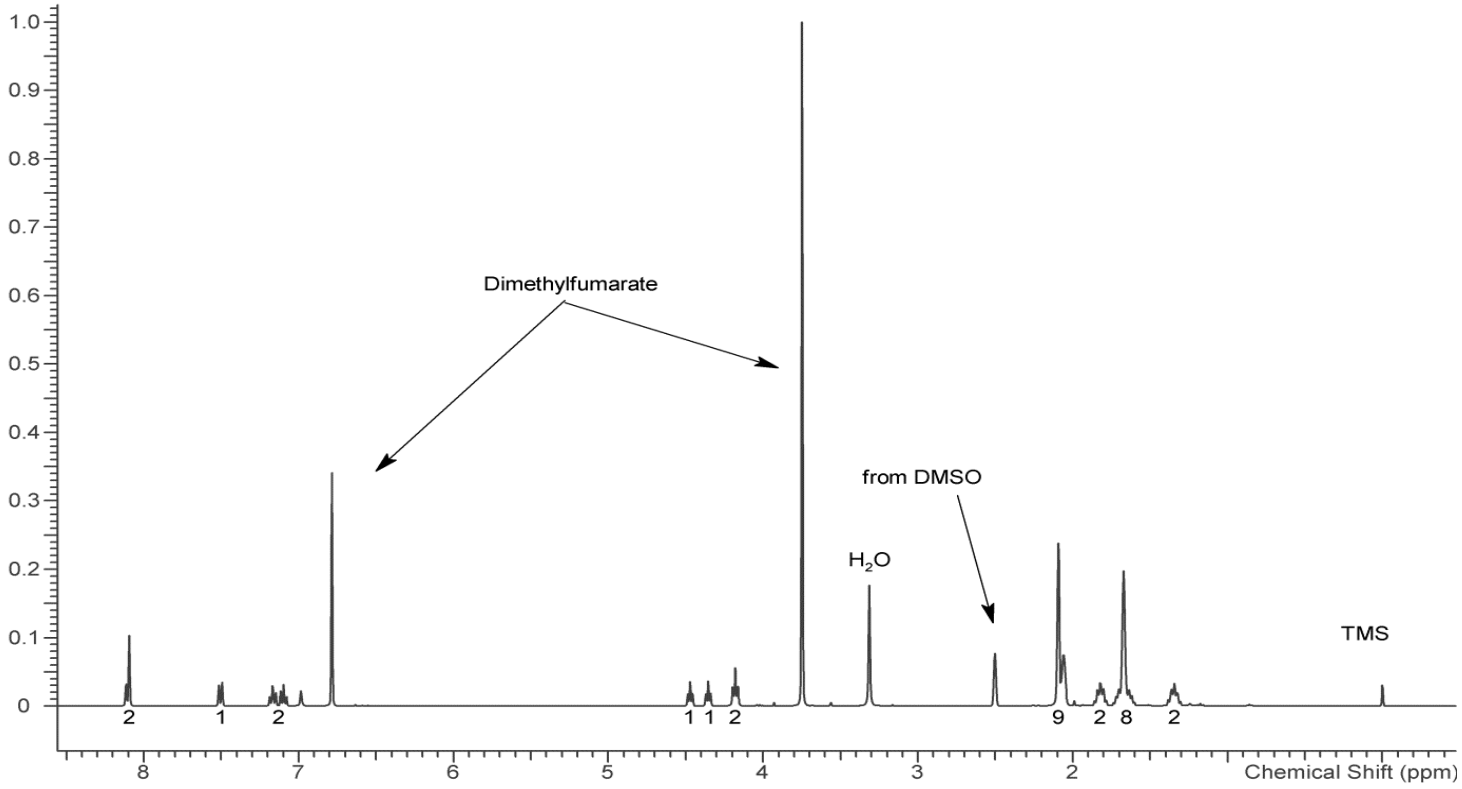
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR DMSO-d_6

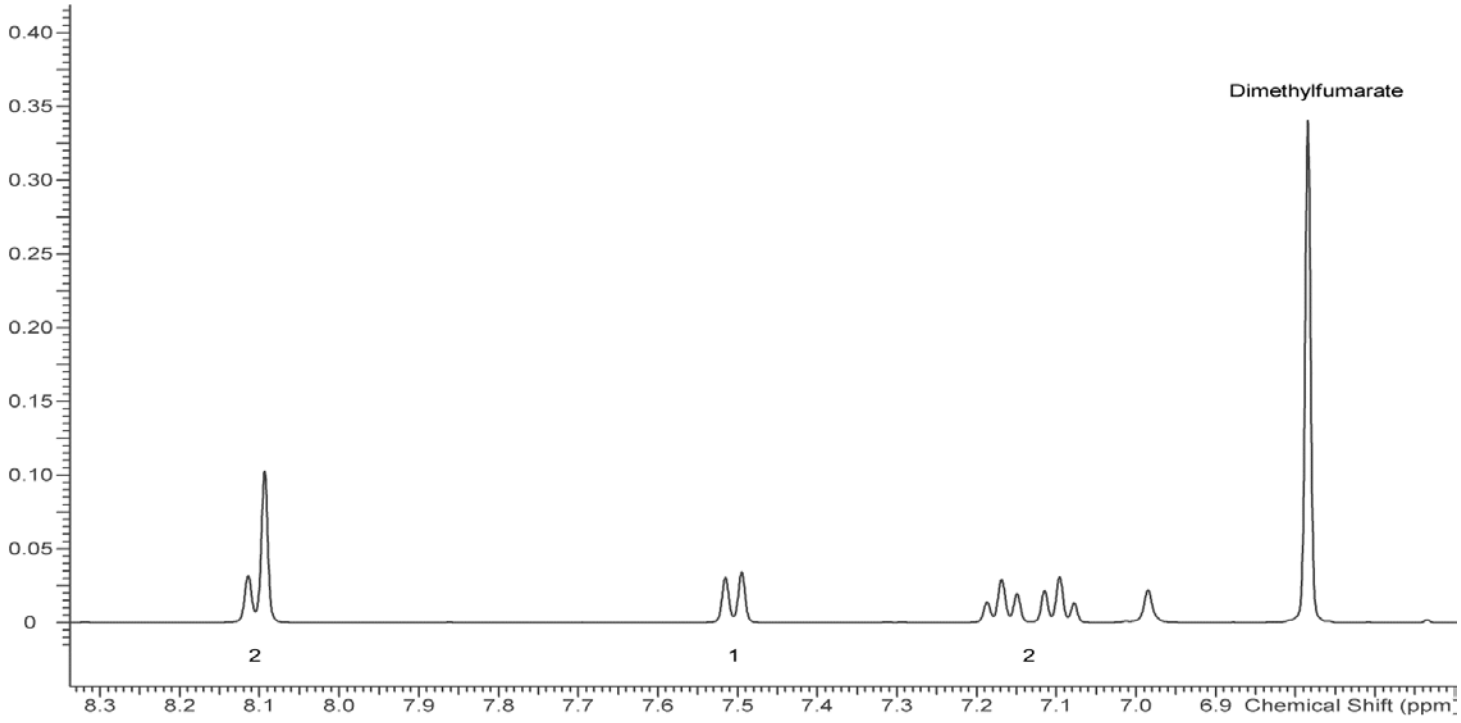
Sample Preparation: Dilute analyte to ~10 mg/mL in DMSO-d_6 containing TMS for 0 ppm reference and dimethylfumarate as quantitative ISTD

Instrument:	Varian Mercury 400 MHz NMR spectrometer with proton detection probe
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm Pulse angle: 90° Delay between pulses: 45 seconds Number of scans (NT): 8 Number of steady state scans: 0 Oversampling: 4 or more Shimming: automatic gradient shimming of Z1-4 shims Phasing, Drift Correction: automatic or manual

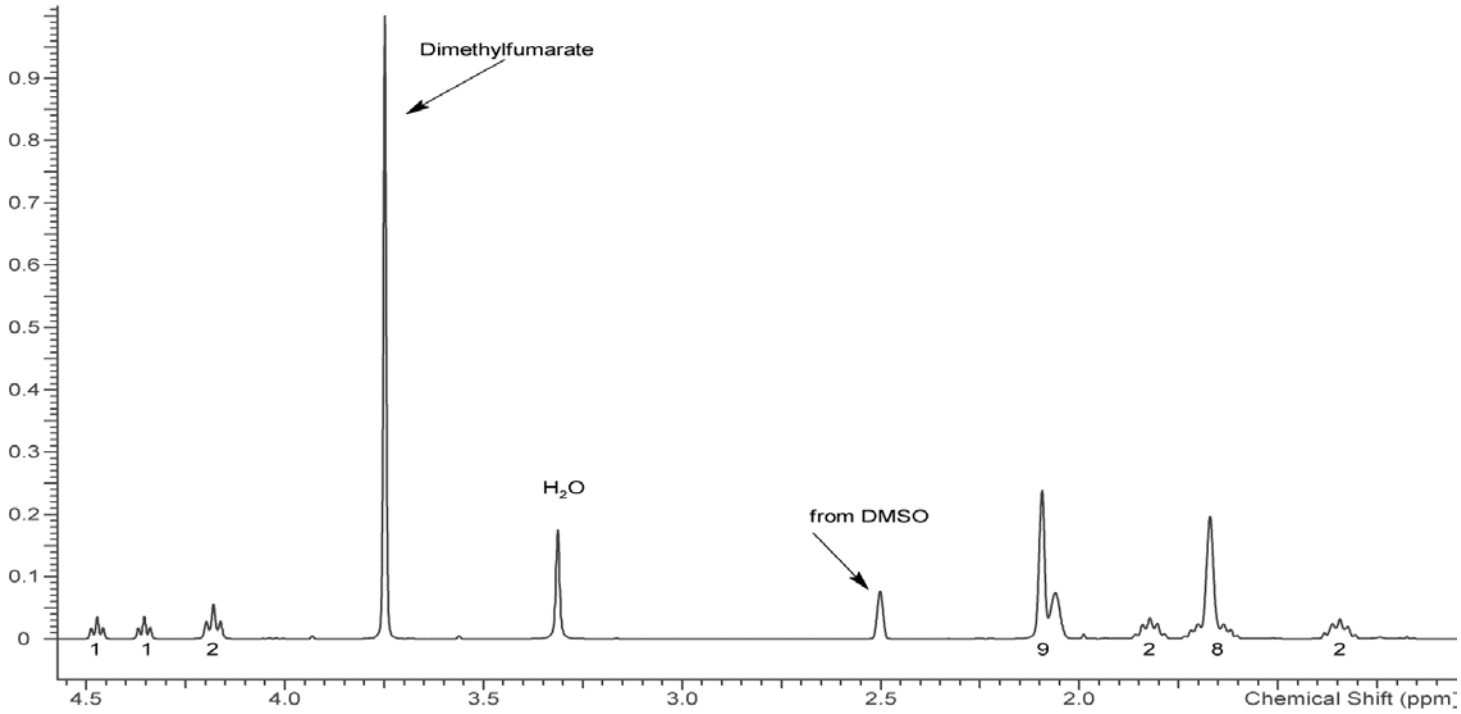
1H NMR: STS-135 Lot # 0436854-17; DMSO; 400MHz



1H NMR: STS-135 Lot # 0436854-17; DMSO; 400MHz



1H NMR: STS-135 Lot # 0436854-17; DMSO; 400MHz

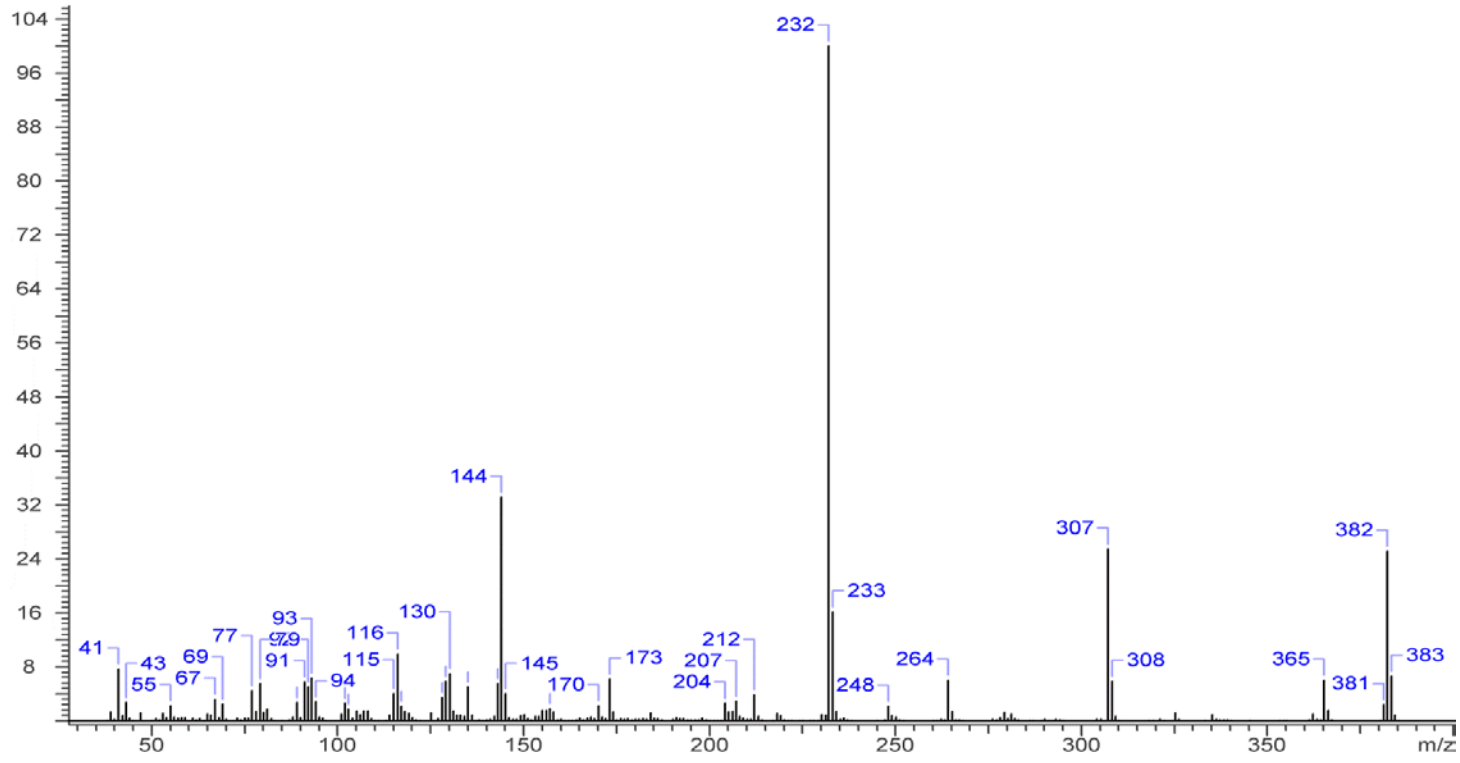


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm
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: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	23.737 minutes

EI Mass Spectra: STS-135 Lot # 0436854-17



3.3 INFRARED SPECTROSCOPY (FTIR)

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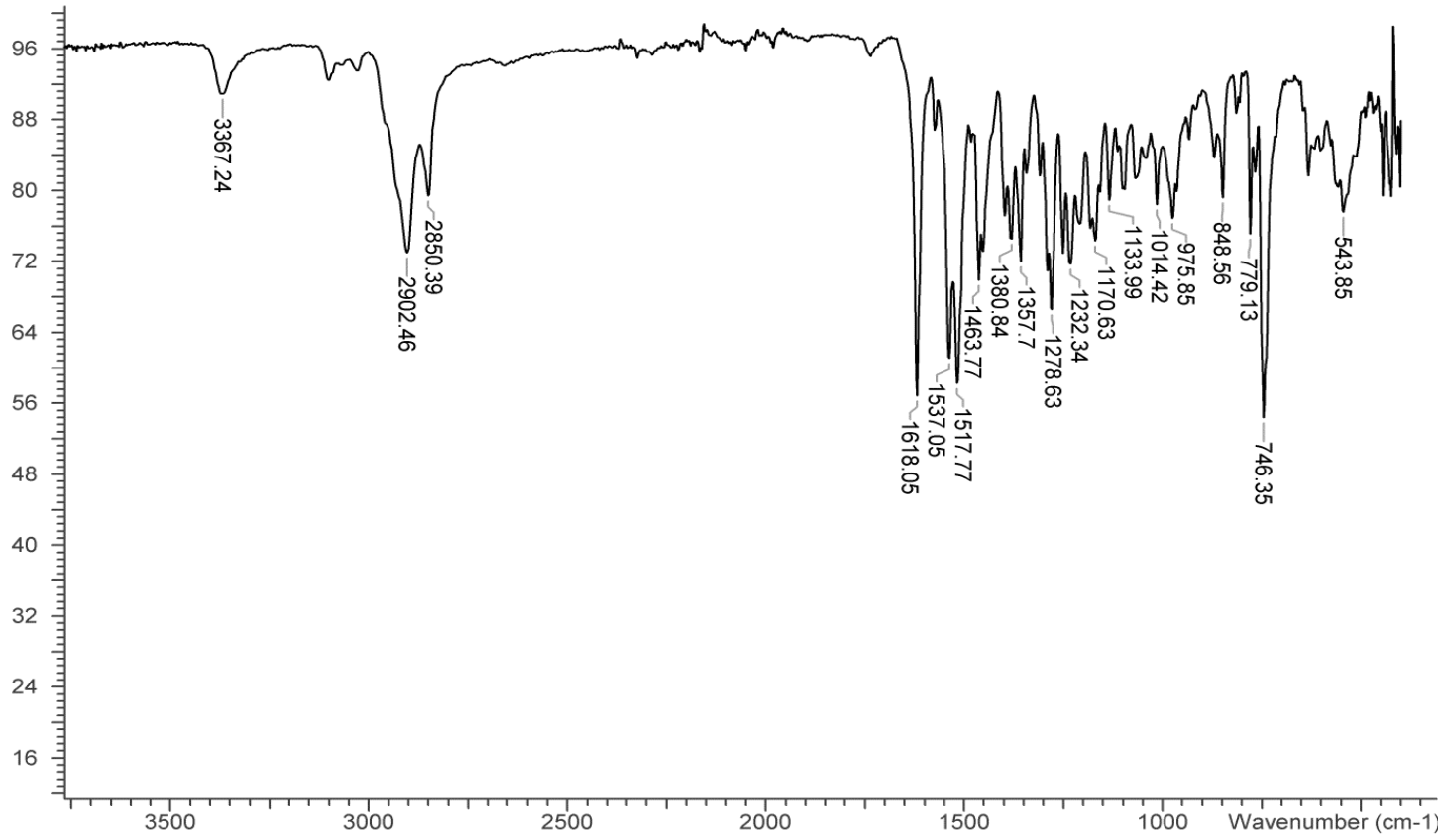
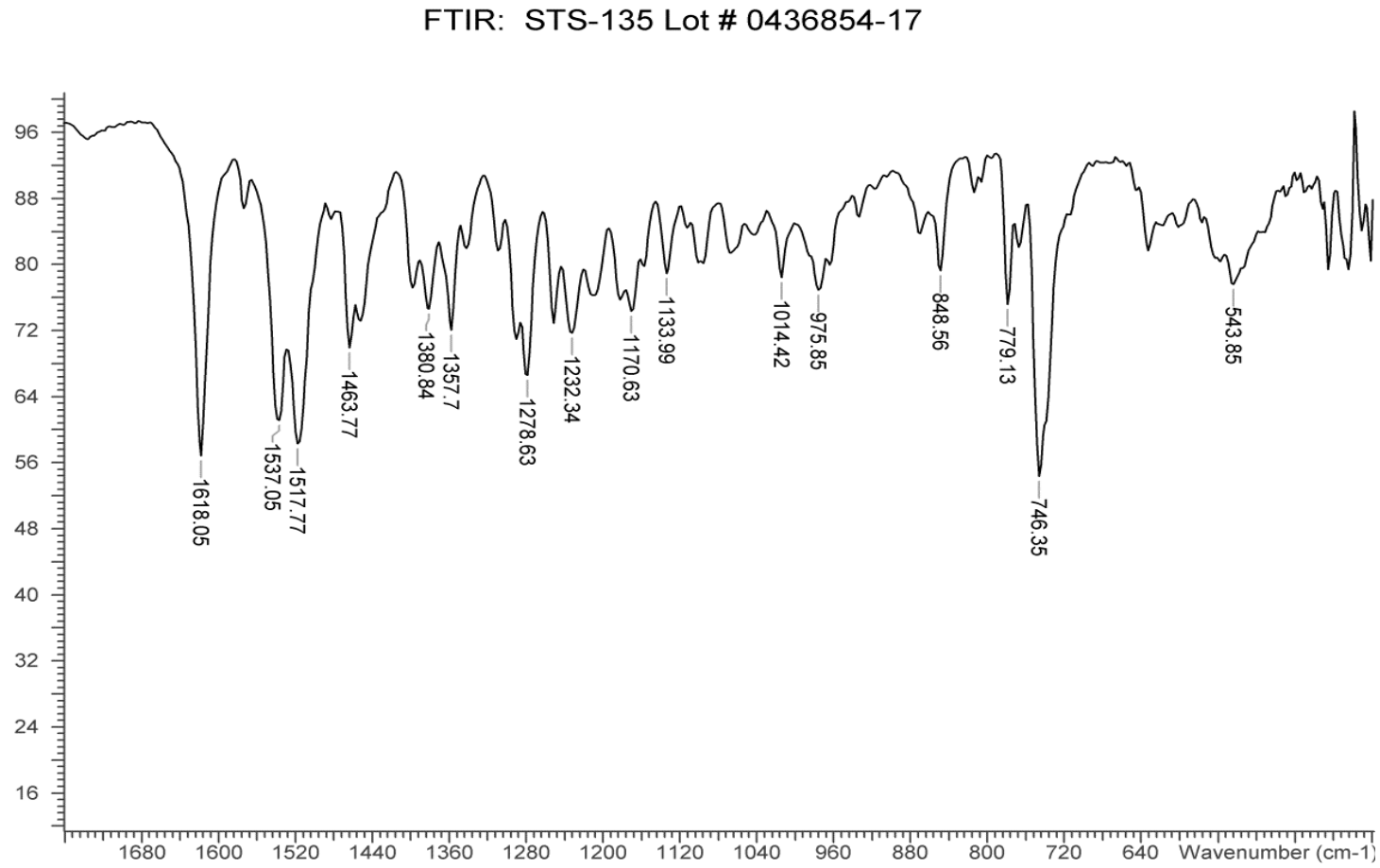
Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR: STS-135 Lot # 0436854-17





4. ADDITIONAL RESOURCES

Forendex