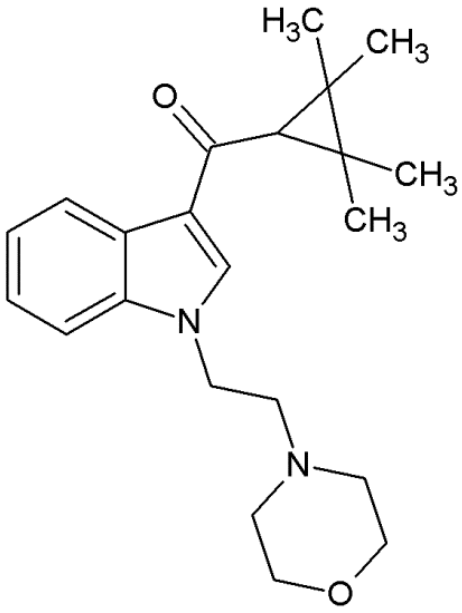


1. GENERAL INFORMATION

IUPAC Name:	{1-[2-(morpholin-4-yl)ethyl]-1H-indol-3-yl}(2,2,3,3-tetramethylcyclopropyl)methanone
CFR:	Not Scheduled (12/2012)
CAS #:	895155-26-7
Synonyms:	NA
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UV_{max}:	215.1, 242.6, 299.7 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{22}H_{30}N_2O_2$	354	134.6

3. ADDITIONAL RESOURCES

Wikipedia

4. QUALITATIVE DATA

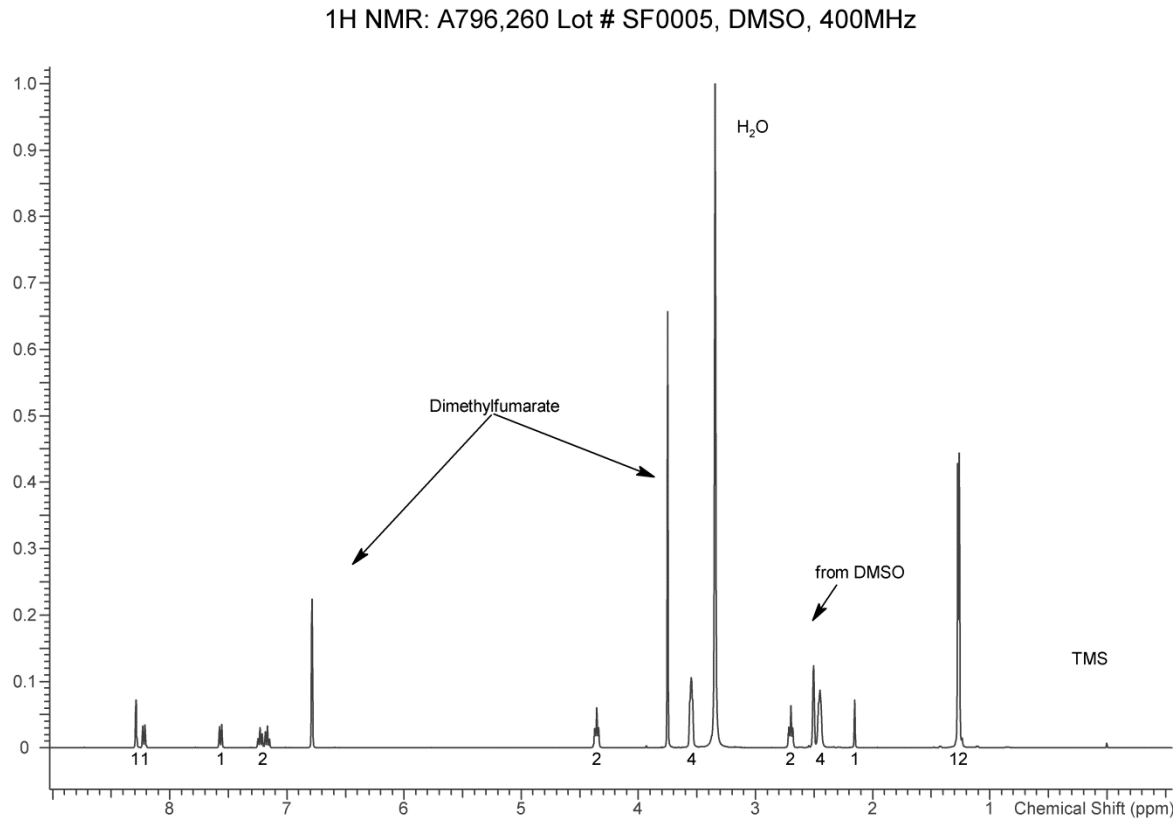
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR DMSO

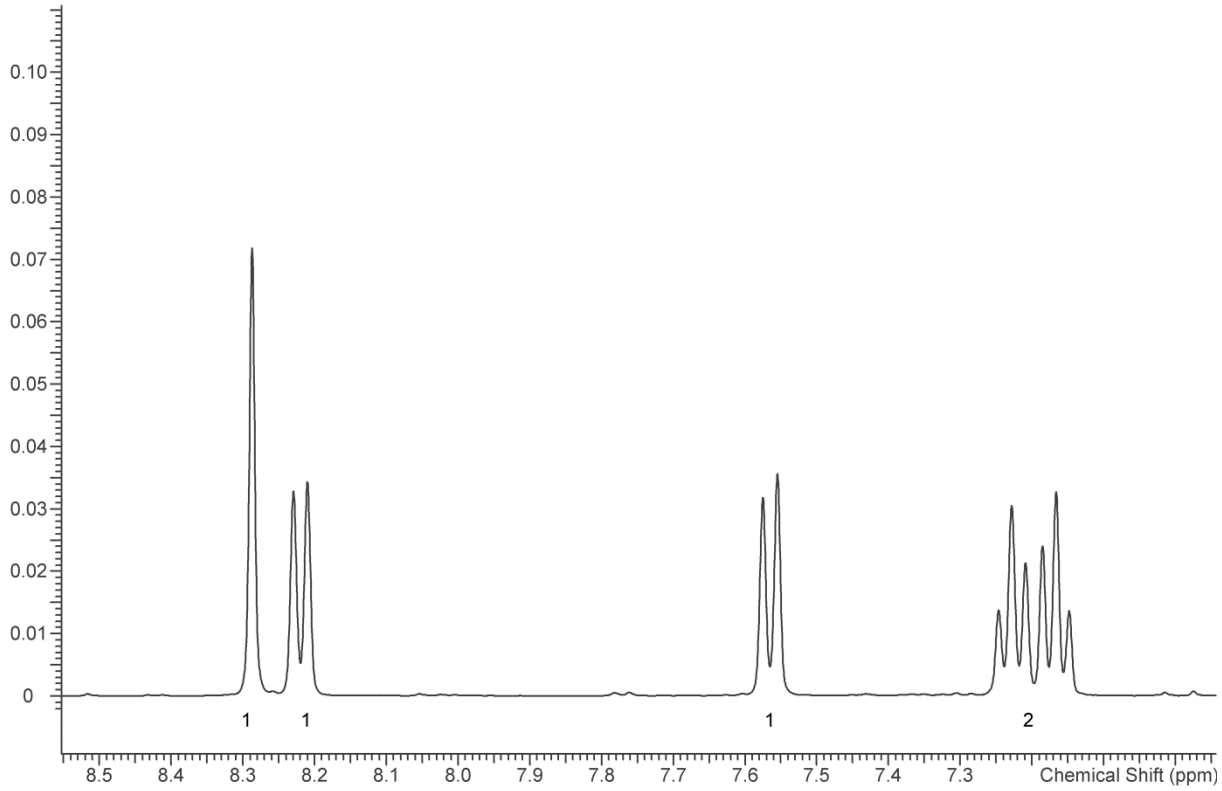
Sample Preparation: Dilute analyte to ~10 mg/mL in DMSO containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

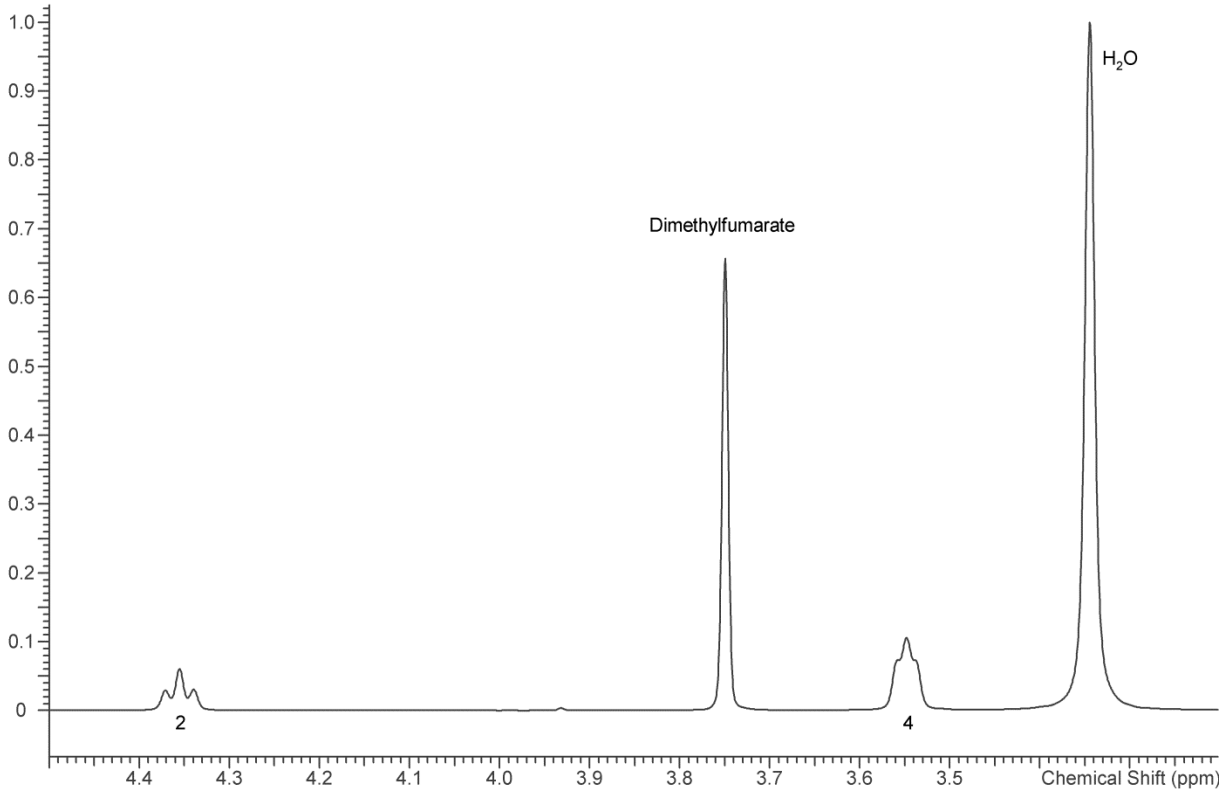
Parameters:
Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual

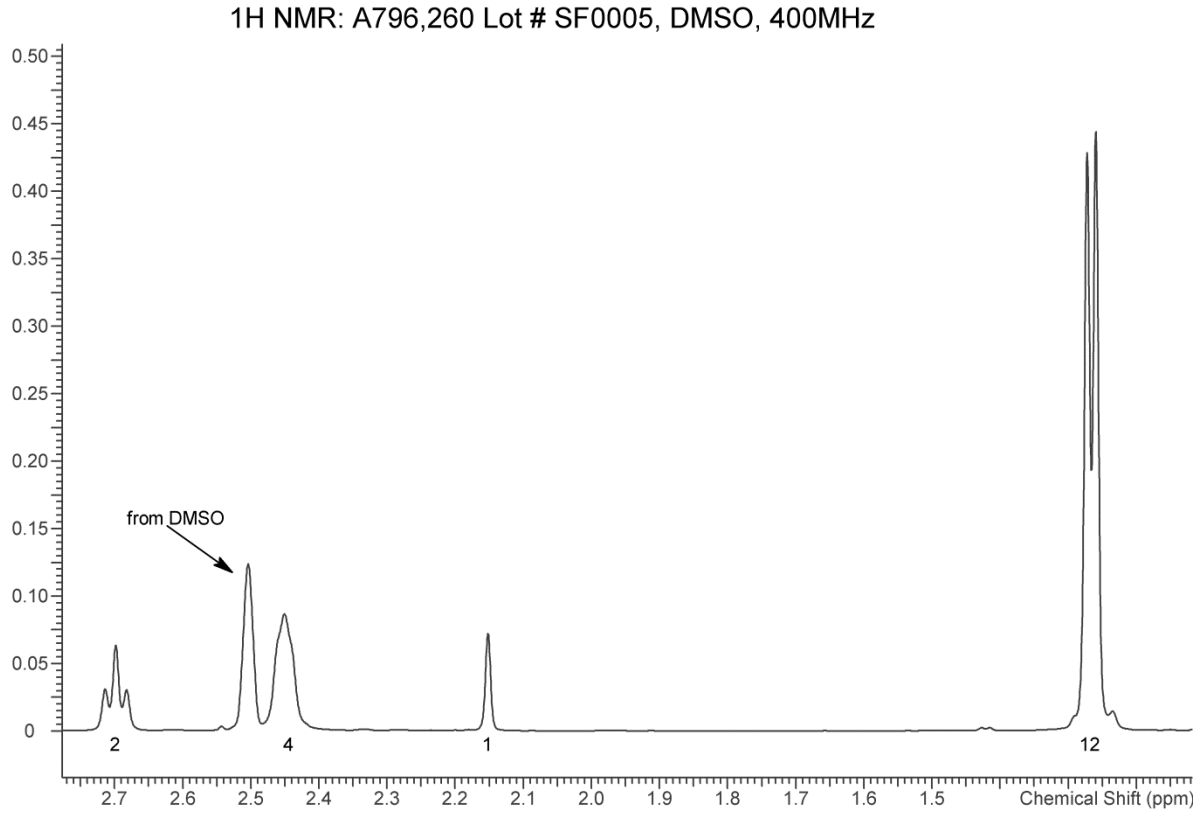


1H NMR: A796,260 Lot # SF0005, DMSO, 400MHz



1H NMR: A796,260 Lot # SF0005, DMSO, 400MHz



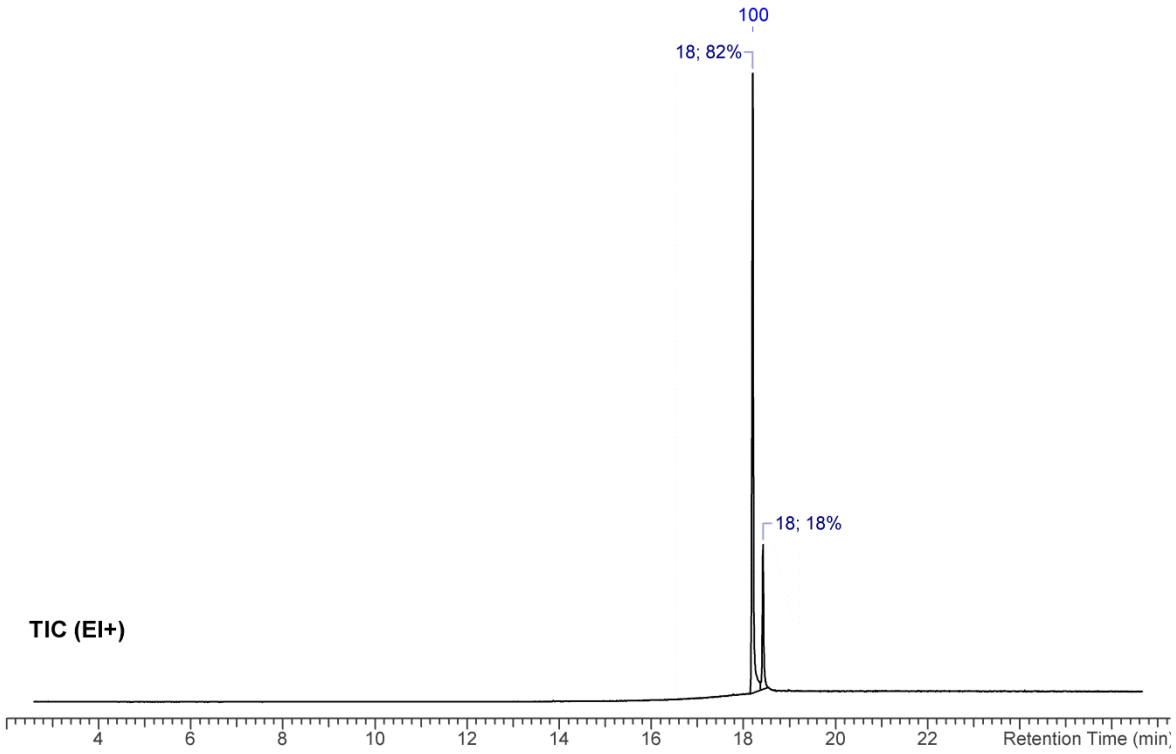


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

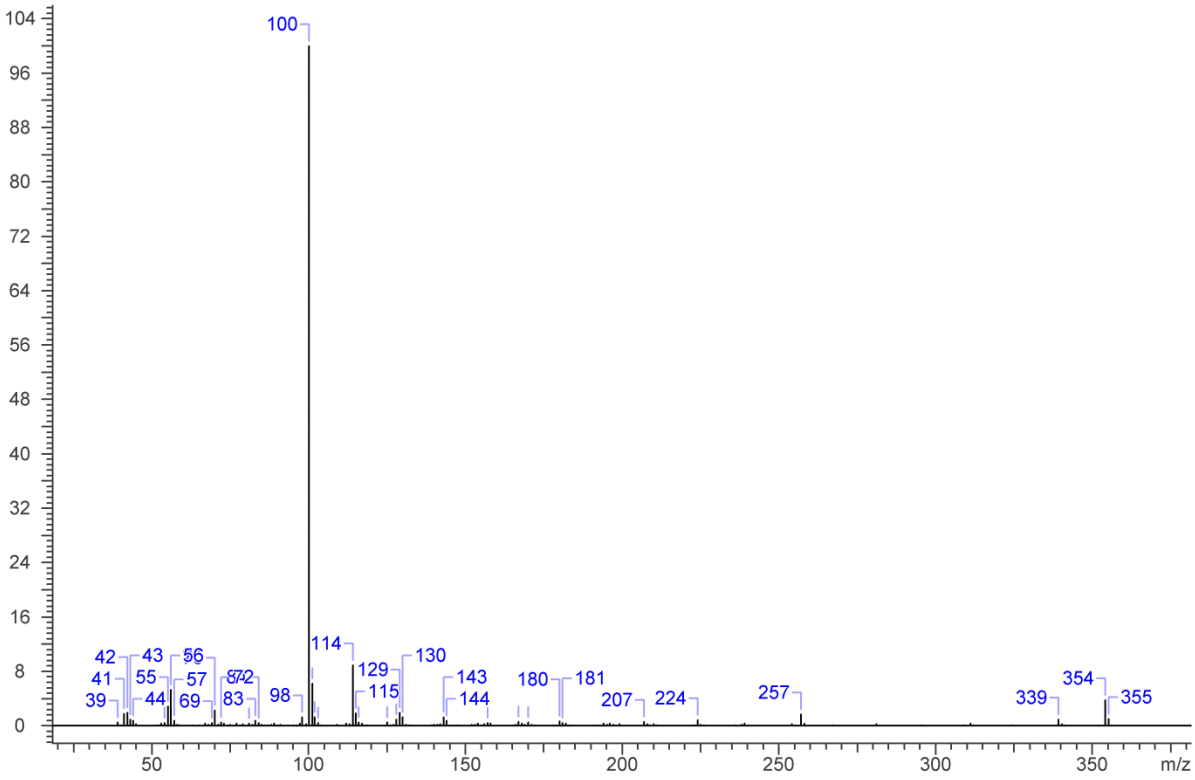
Sample Preparation: Dilute analyte to ~1 mg/mL in $CHCl_3$.

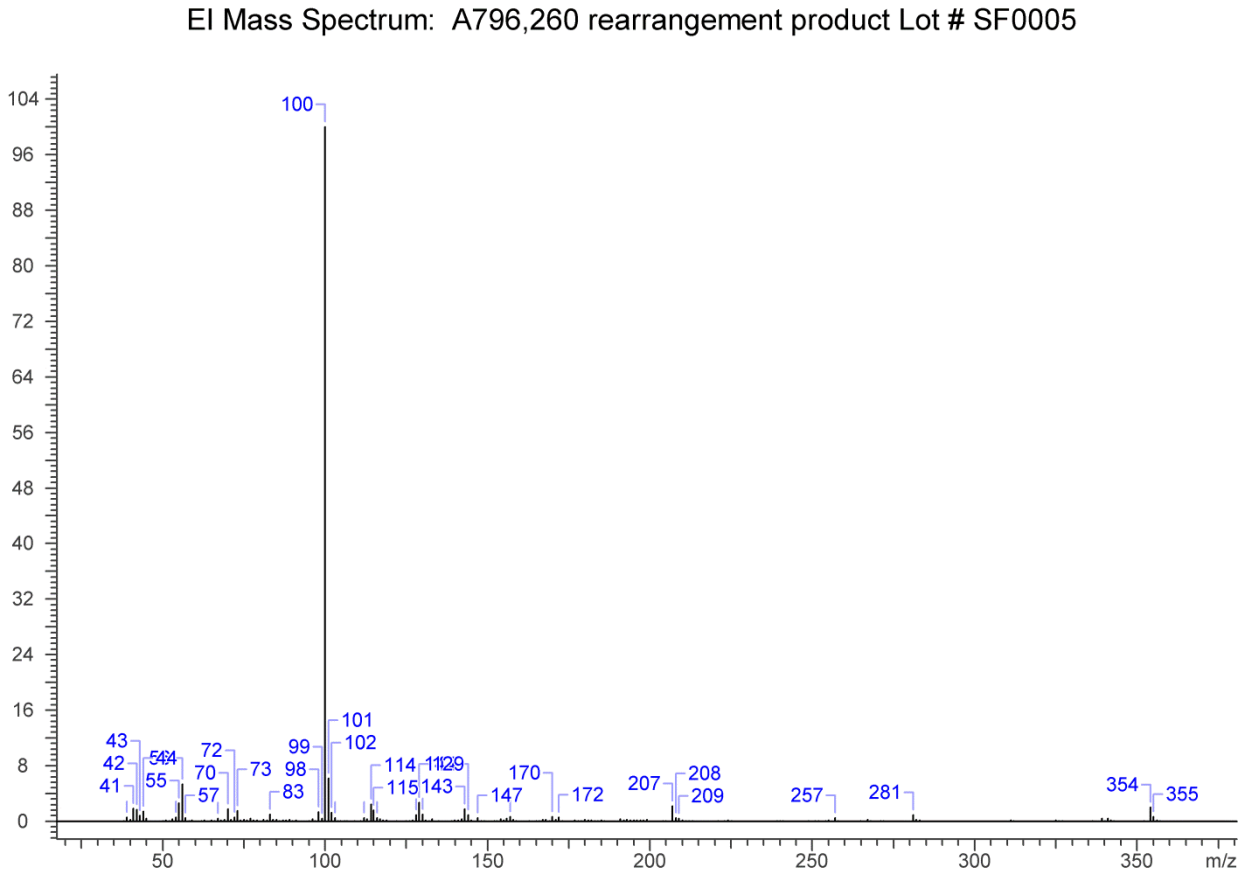
Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS; 30m x .25mm x .25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C 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: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	A796,260 peak at 18.202 min; Rearrangement peak at 18.426 min

GC/MS TIC: A796,260 Lot # SF0005



EI Mass Spectrum: A796,260 Lot # SF0005





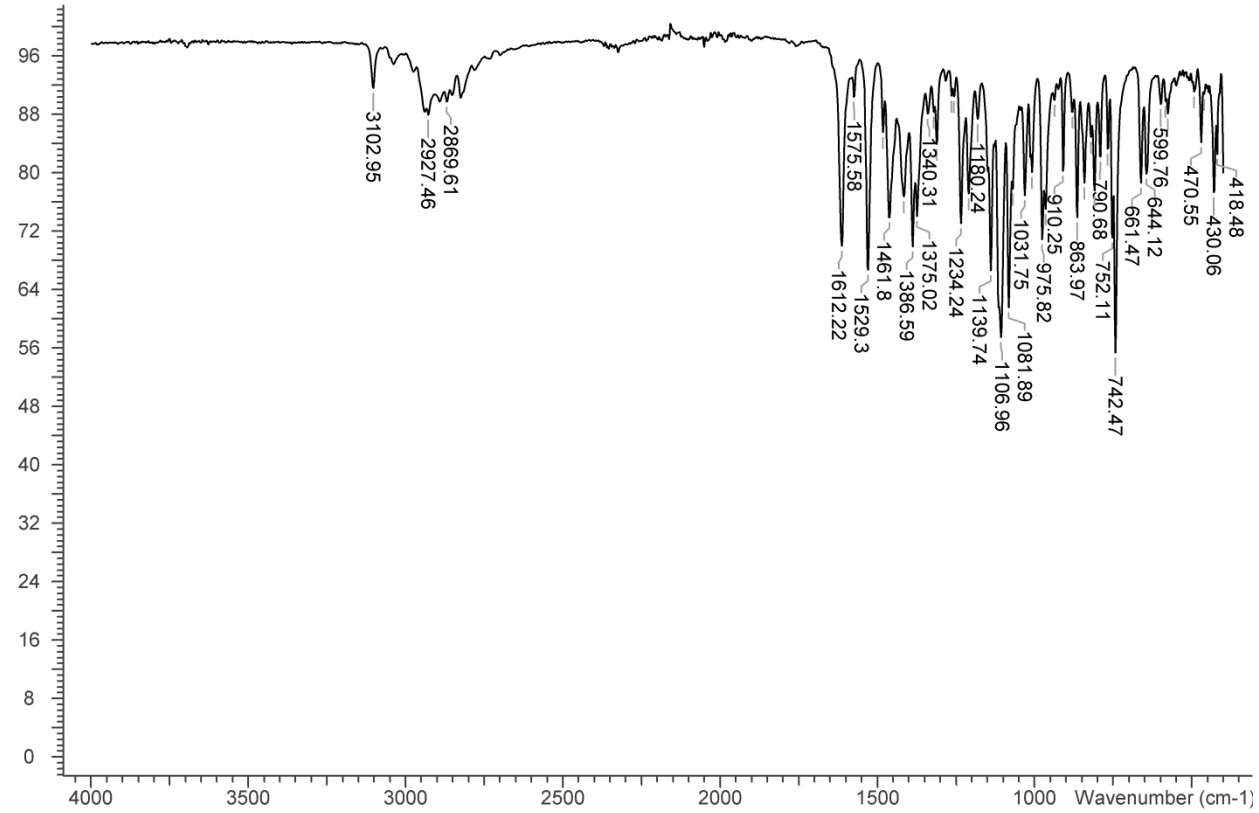
GC/MS Analytical Observation:

The GC/MS TIC of A796,260 shows two peaks with similar mass spectra (shown above). The major peak at retention time 18.202 minutes is A796,260; while the minor peak at retention time 18.426 minutes is a thermally induced rearrangement product of A796,260. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.

4.3 INFRARED SPECTROSCOPY (FTIR)

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 ATR (Diamond, 3 Bounce): A796,260 Lot # SF0005



FTIR ATR (Diamond, 3 Bounce): A796,260 Lot # SF0005