

1. GENERAL INFORMATION

IUPAC Name:	[1-(5-chloropentyl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone
CFR:	Not Scheduled (12/2012)
CAS #:	Not Available
Synonyms:	UR-144 N-(5-chloropentyl) analog
Source:	DEA Reference Material Collection
Appearance:	White Powder
Kovat's Index:	Pending
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₁ H ₂₈ ClNO	345	79.0

3. ADDITIONAL RESOURCES

No resources identified as of 12/28/2012.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

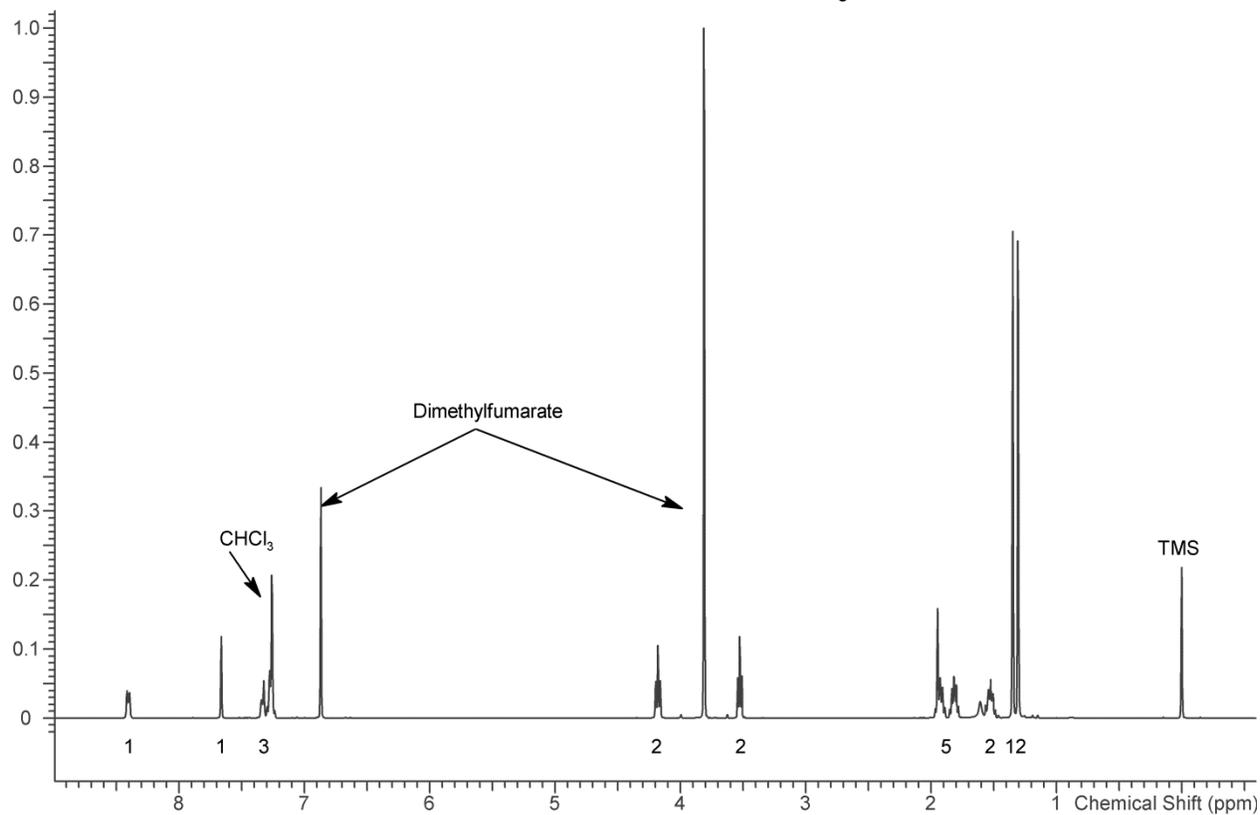
Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~5 mg/mL in deuteriochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

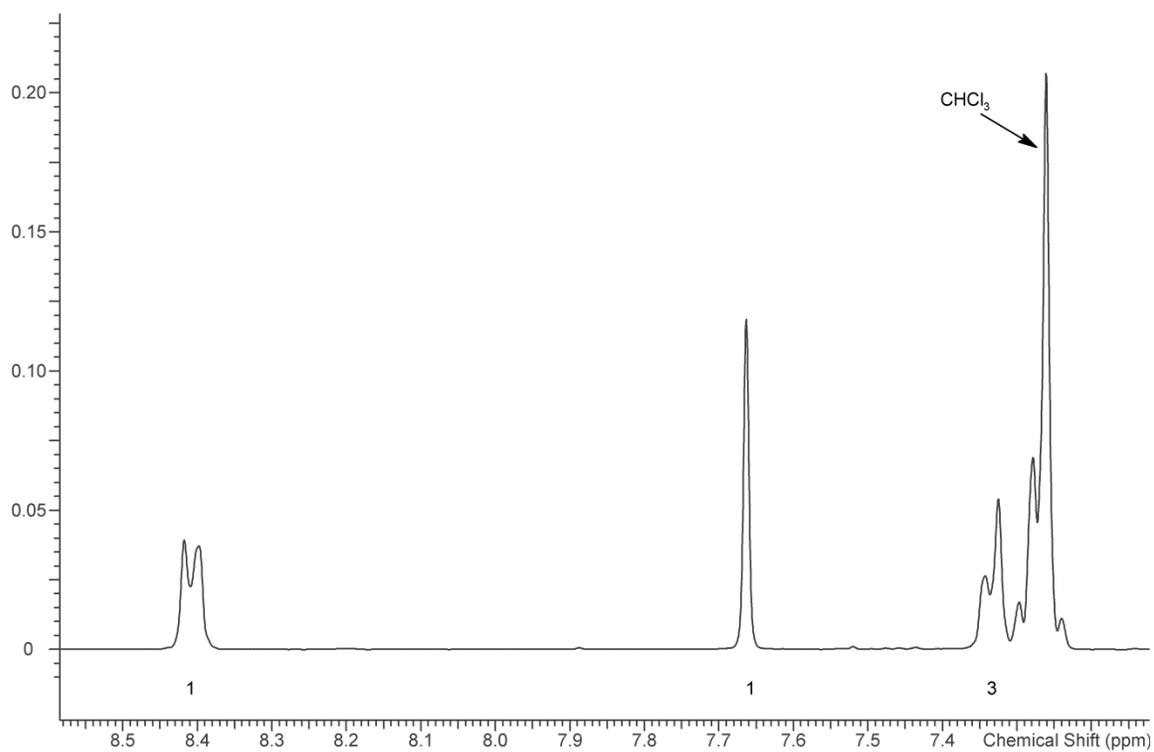
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

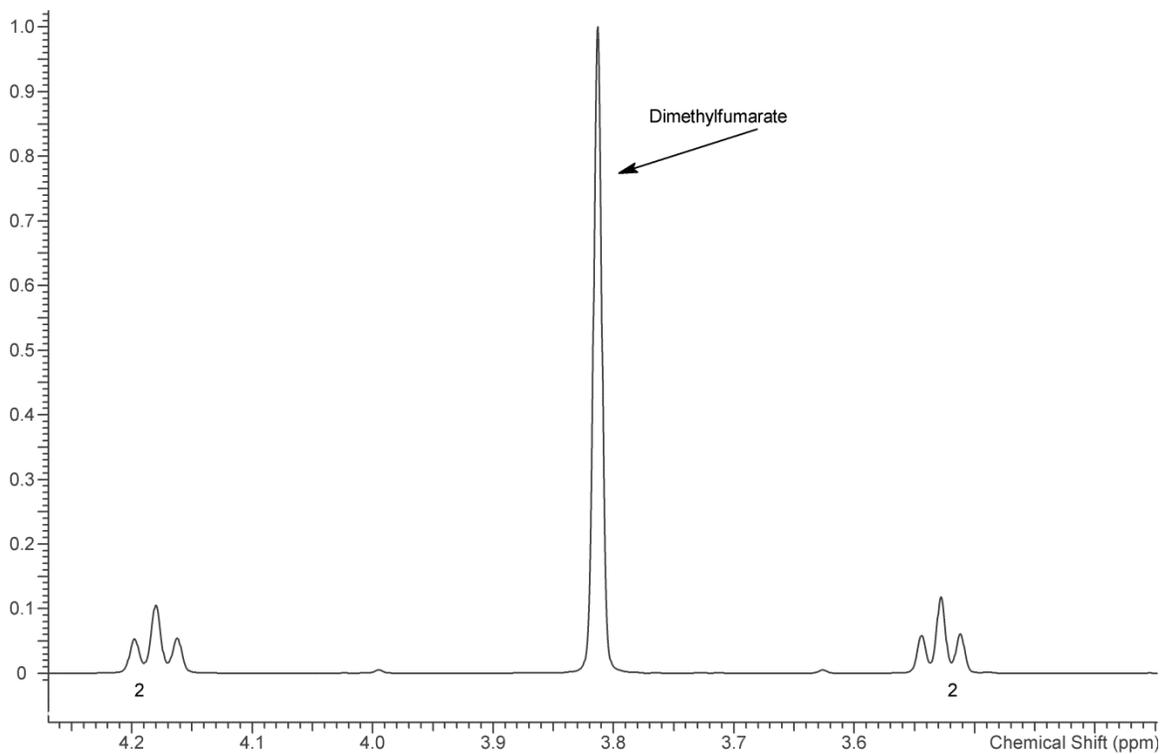
1H NMR: 5-Chloro-UR-144 Lot # 0441217-10; CDCl₃; 400 MHz



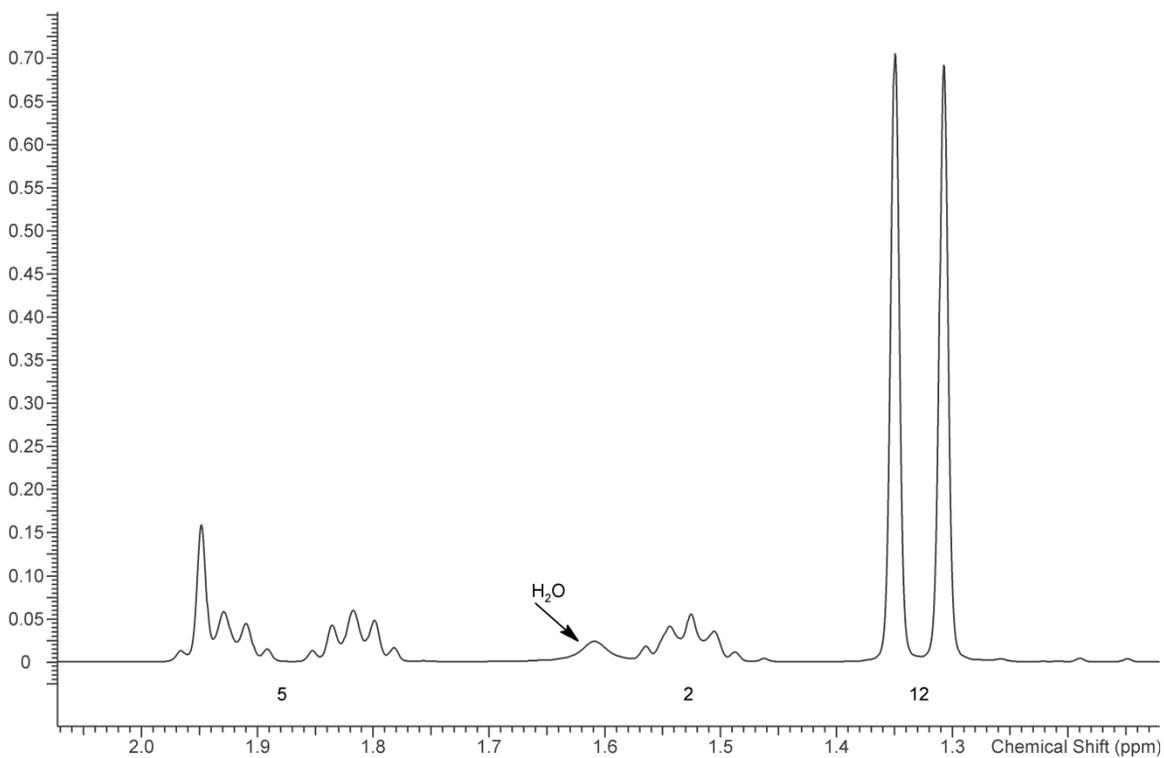
1H NMR: 5-Chloro-UR-144 Lot # 0441217-10; CDCl₃; 400 MHz



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1H NMR: 5-Chloro-UR-144 Lot # 0441217-10; CDCl₃; 400 MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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

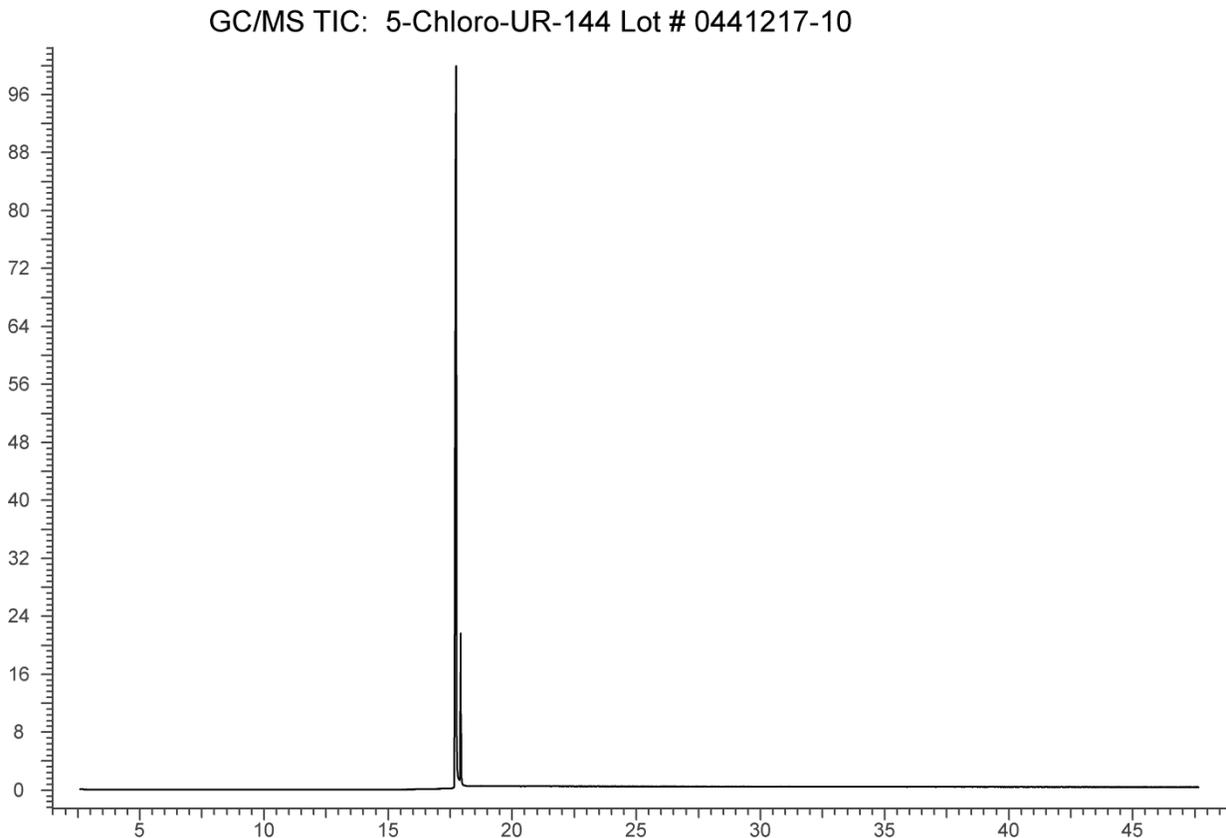
MS Parameters: Mass scan range: 30-550 amu

Threshold: 100

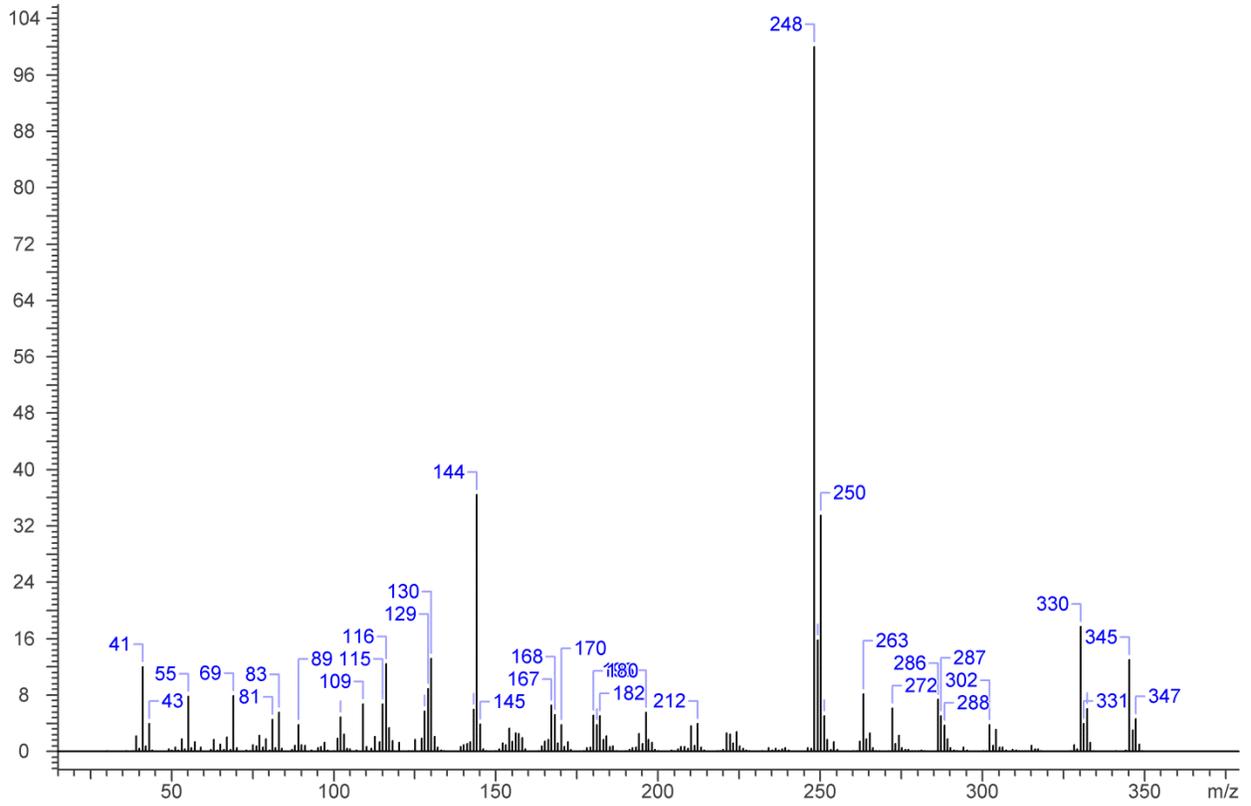
Tune file: stune.u

Acquisition mode: scan

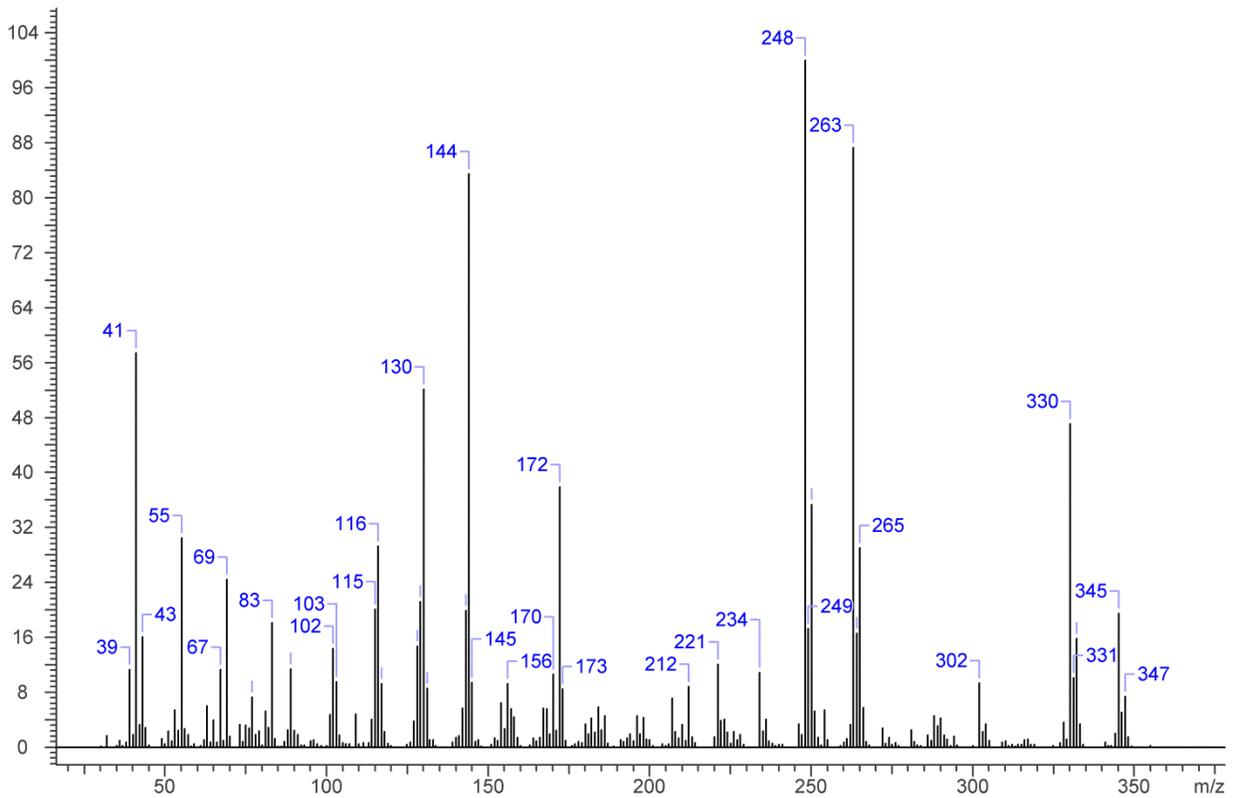
Retention Time: 5-Cl-UR-144 peak at 17.728 min; Rearrangement peak at 17.924 min



EI Mass Spectrum: 5-Chloro-UR-144 Lot # 0441217-10



EI Mass Spectrum: 5-Chloro-UR-144 Rearrangement Lot # 0441217-10



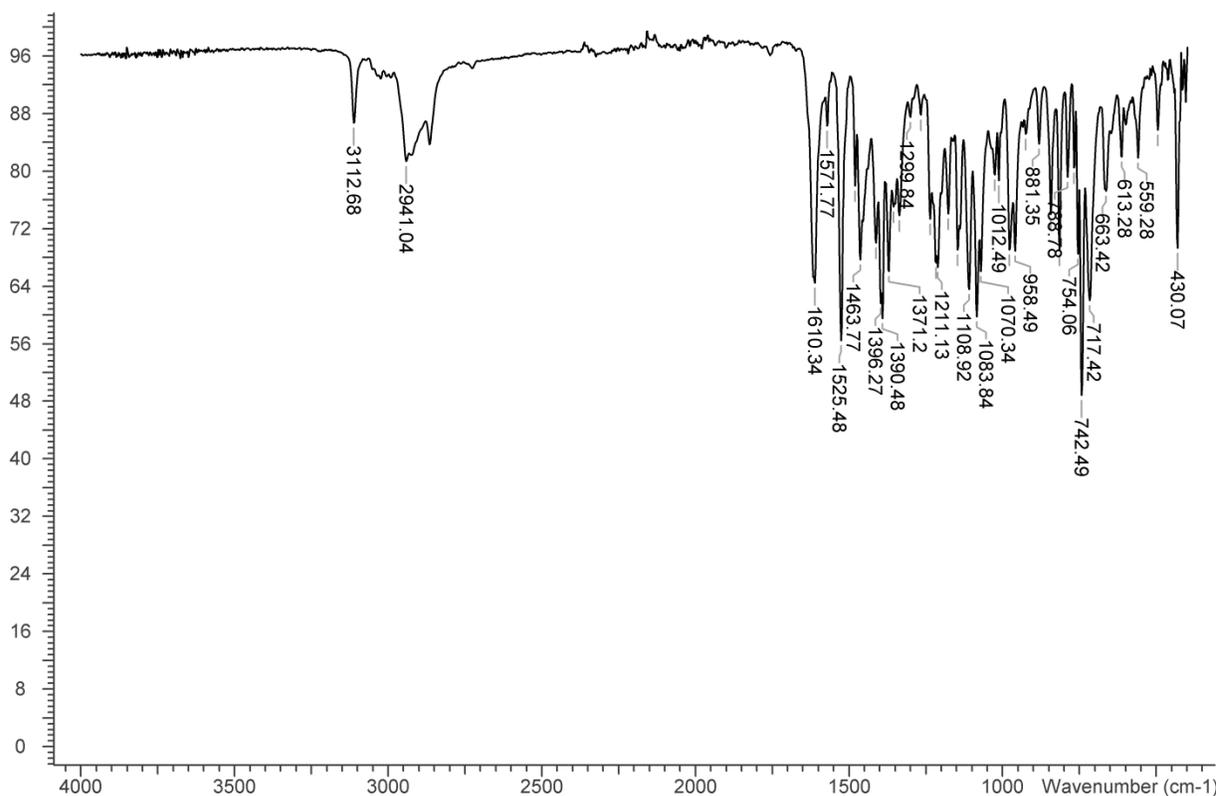
GC/MS Analytical Observation:

The GC/MS TIC of 5-Chloro-UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 17.728 minutes, is 5-Chloro-UR-144 while the minor peak, with a retention time of 17.924 minutes, is a thermally induced rearrangement product of 5-Chloro-UR-144. 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): 5-Cl-UR-144 Lot # 0441217-10



FTIR ATR (Diamond, 3 Bounce): 5-CI-UR-144 Lot # 0441217-10

