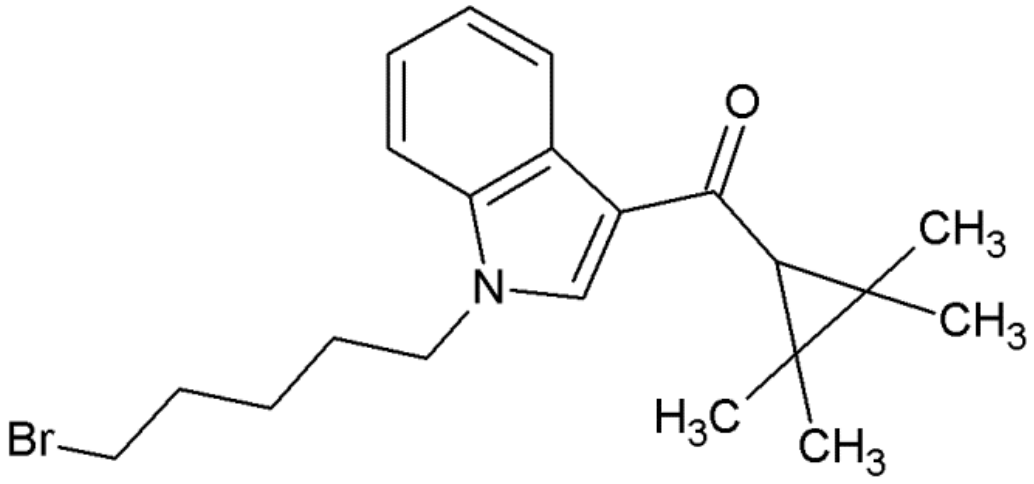


1. GENERAL INFORMATION

IUPAC Name: [1-(5-bromopentyl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone

CFR: Not Scheduled (01/2013)

CAS #: Not Available

Synonyms: UR-144 N-(5-bromopentyl) 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	$C_{21}H_{28}BrNO$	390	93.0

3. ADDITIONAL RESOURCES

No resources identified as of 12/28/2012.

4. QUALITATIVE DATA

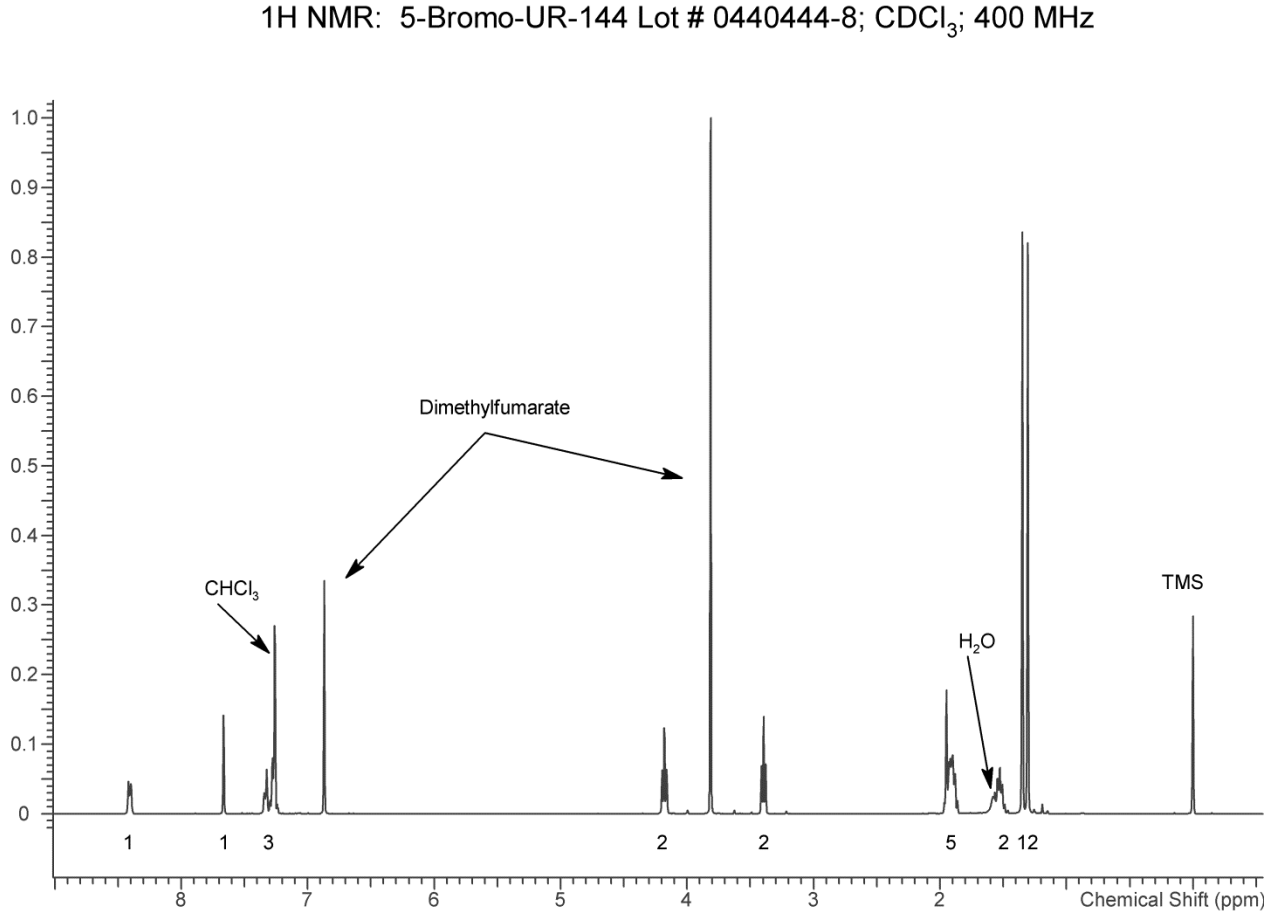
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

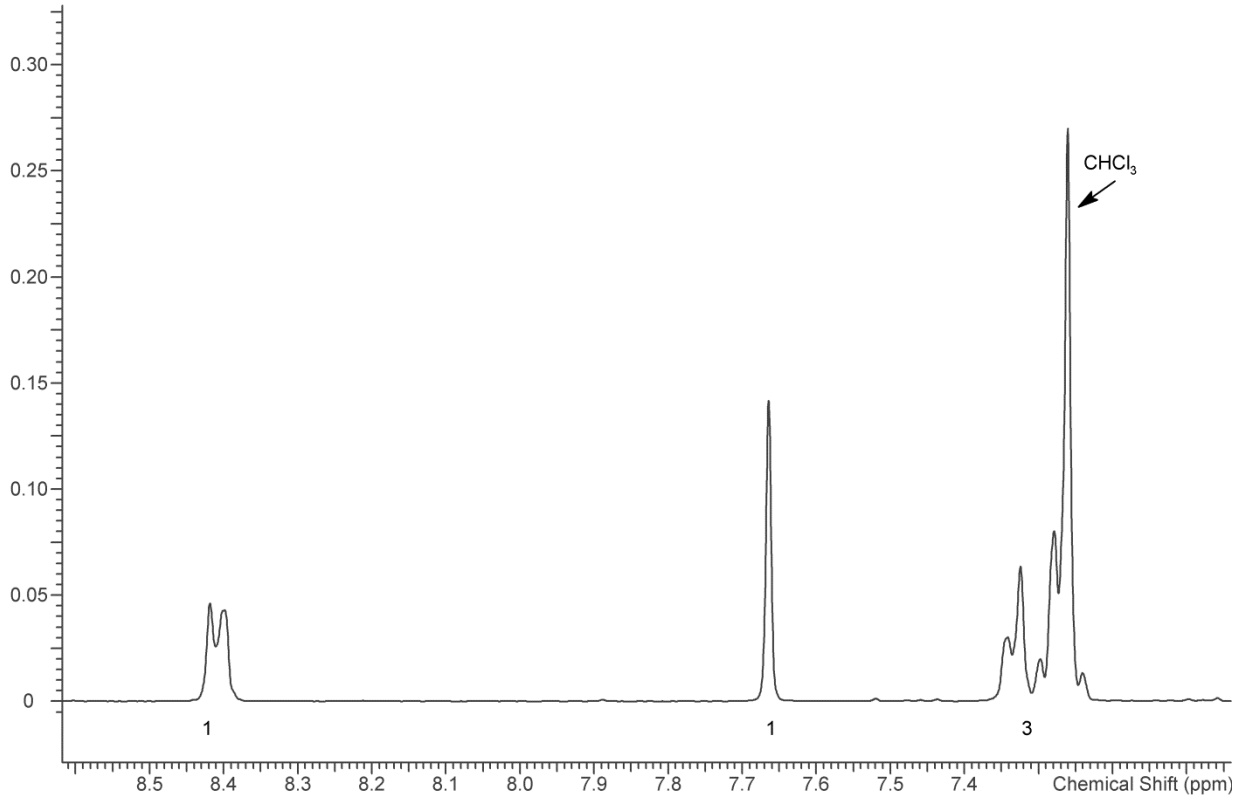
Sample Preparation: Dilute analyte to ~5 mg/mL in deuterochloroform ($CDCl_3$) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

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

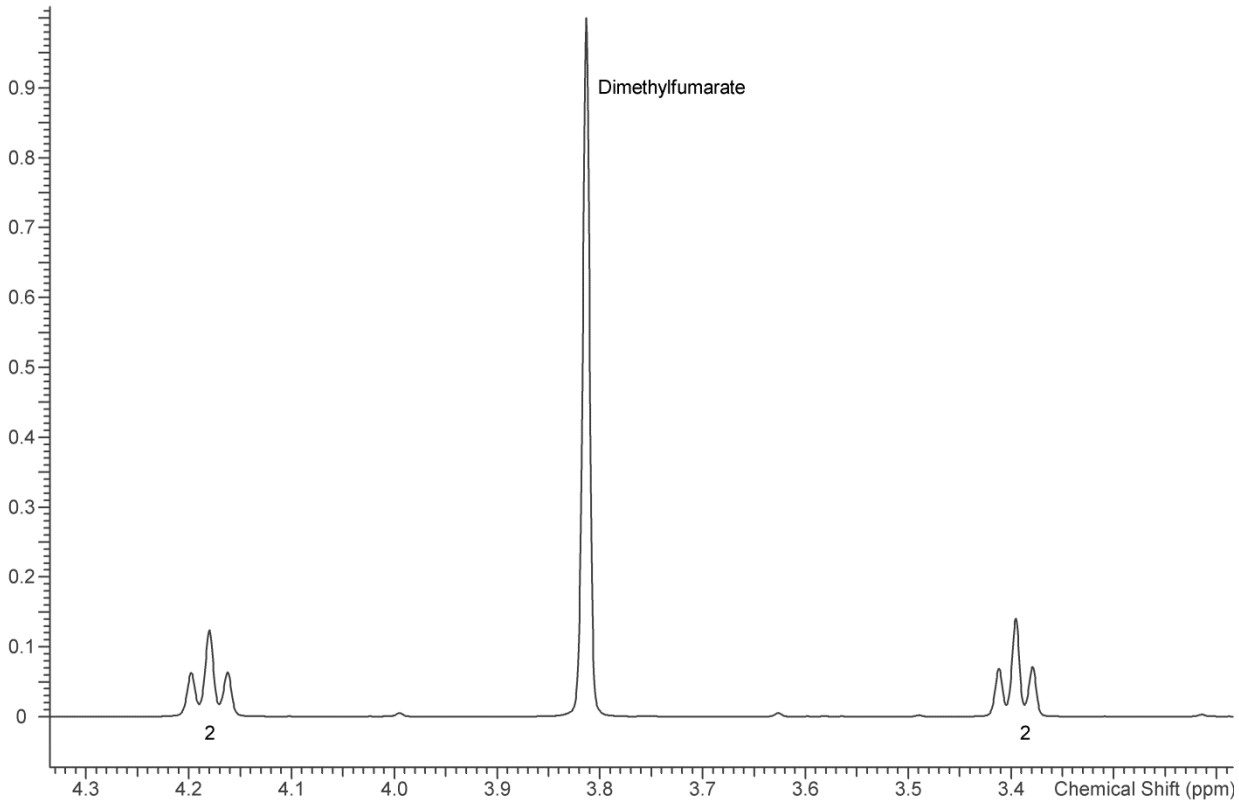
Parameters:
Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual



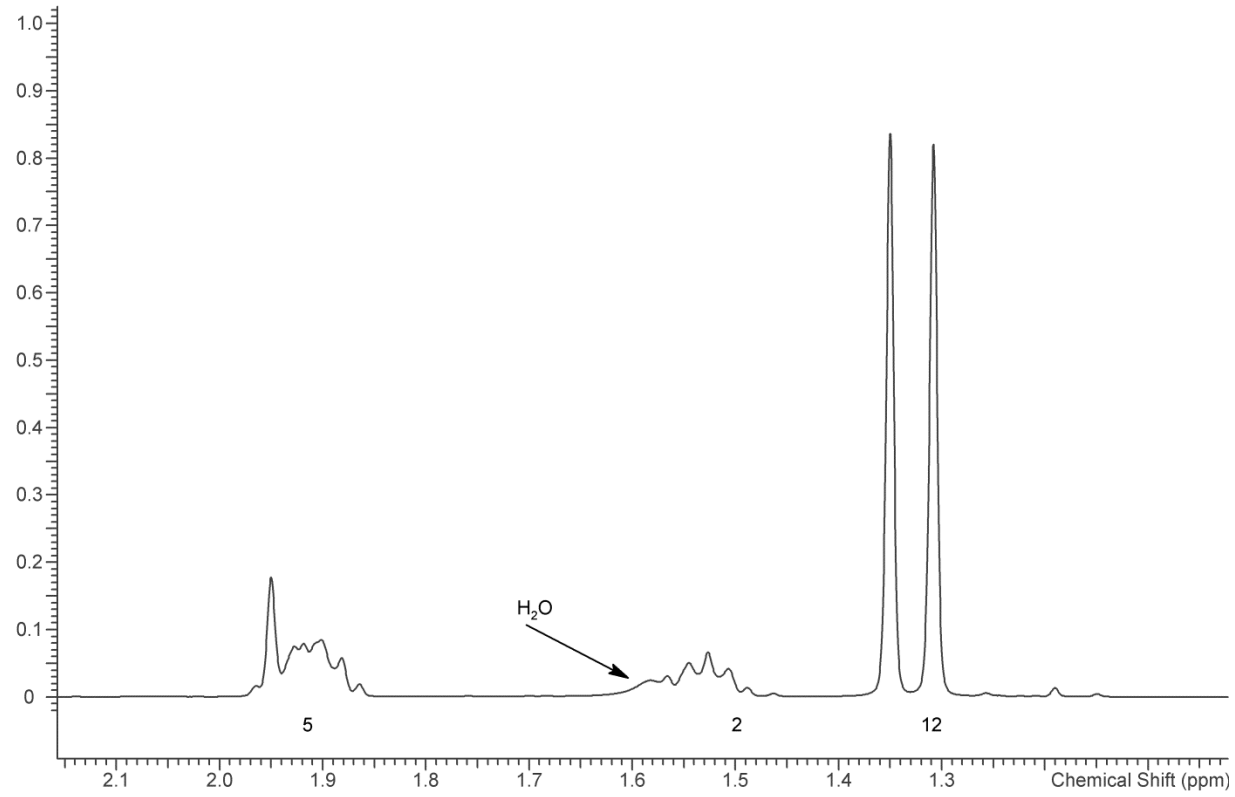
1H NMR: 5-Bromo-UR-144 Lot # 0440444-8; $CDCl_3$; 400 MHz



1H NMR: 5-Bromo-UR-144 Lot # 0440444-8; $CDCl_3$; 400 MHz



1H NMR: 5-Bromo-UR-144 Lot # 0440444-8; $CDCl_3$; 400 MHz

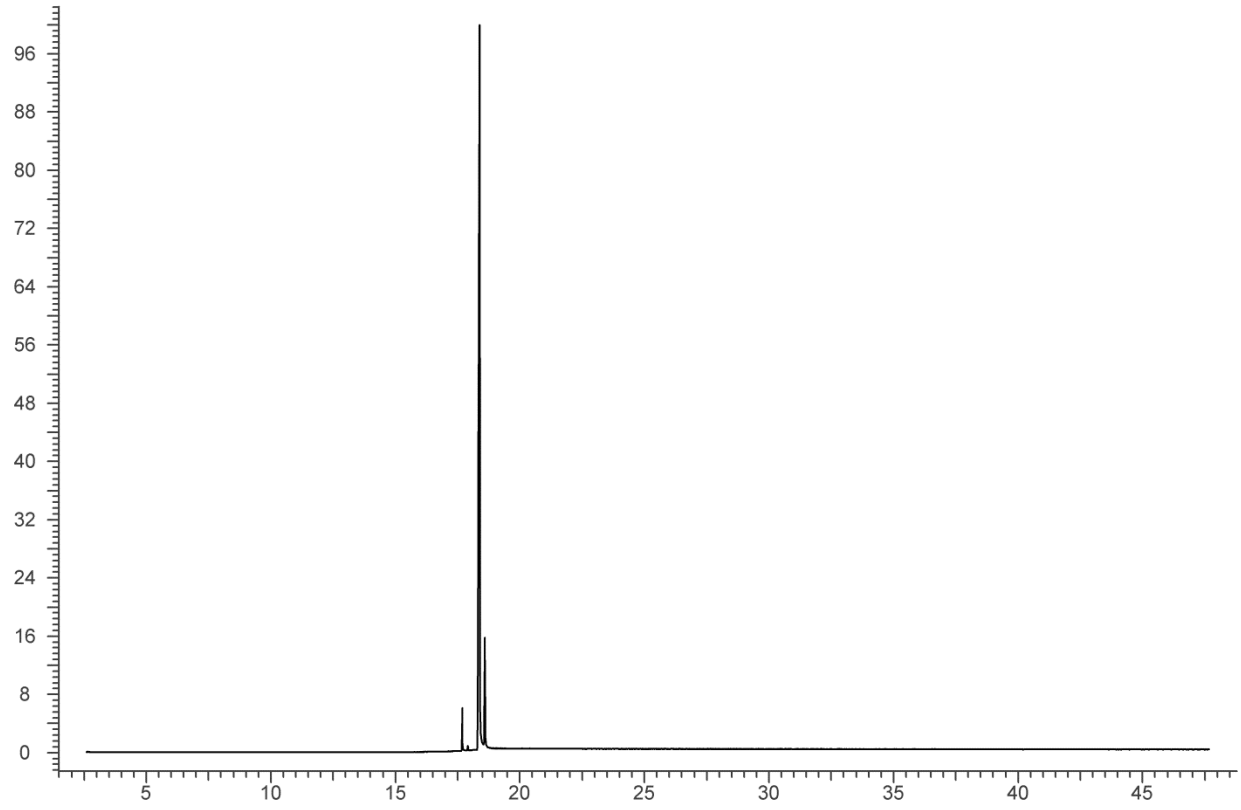


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

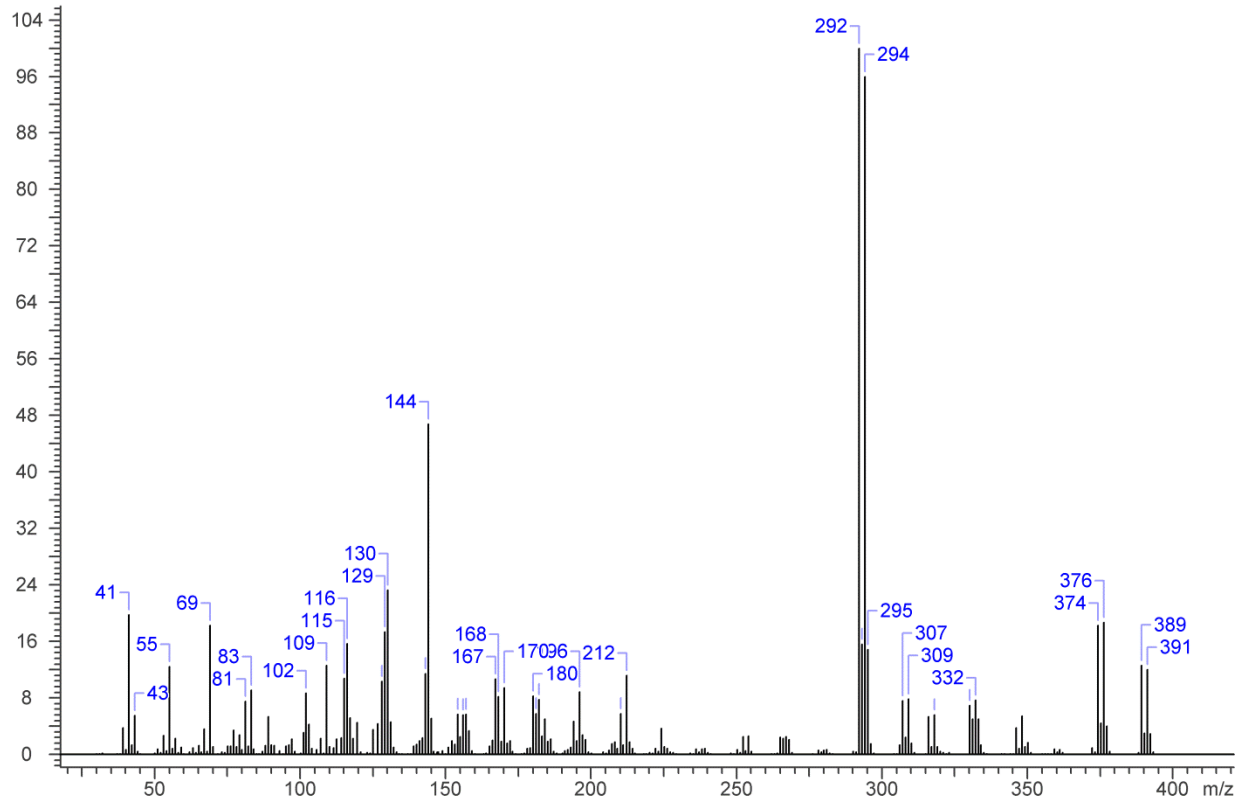
Sample Preparation: Dilute analyte to ~4 mg/mL in $CHCl_3$.

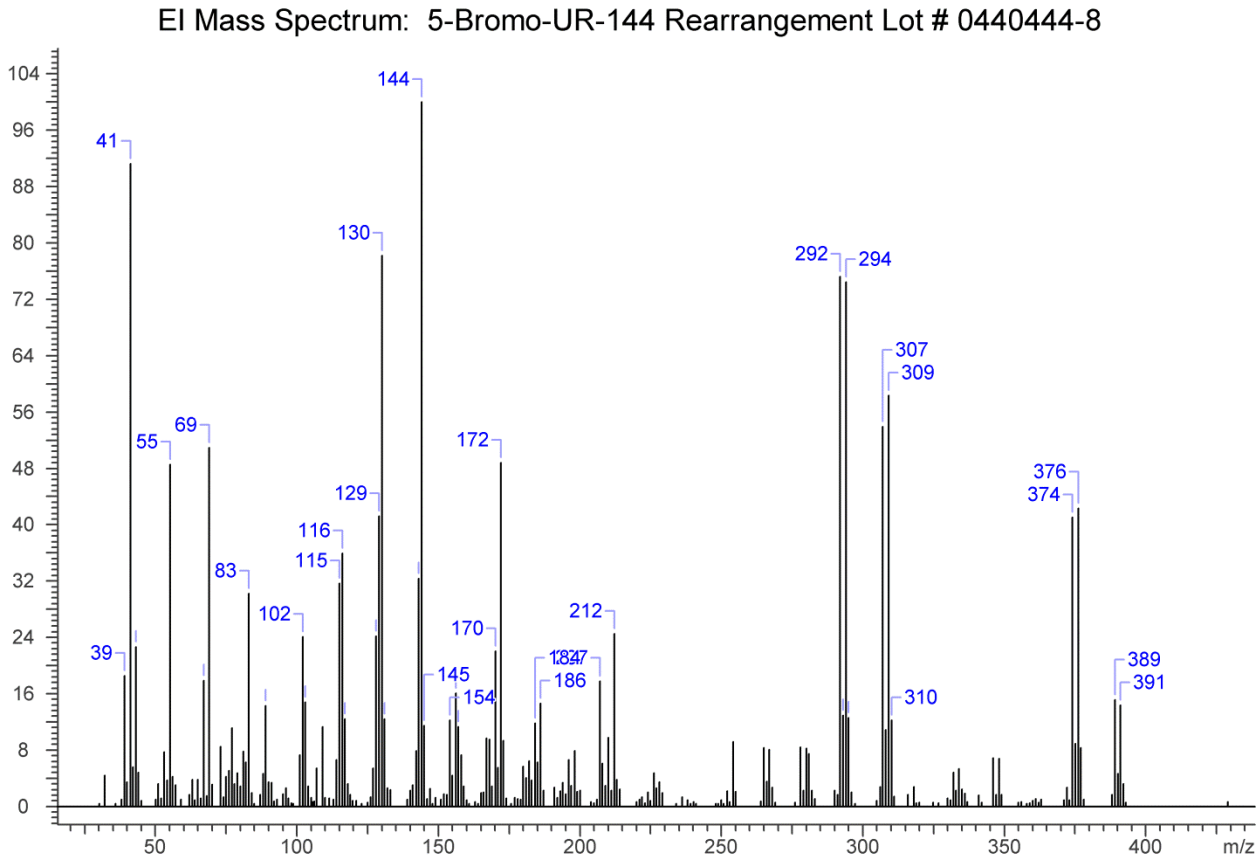
Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS; 30m x .25mm x .25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C 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:	5-Bromo-UR-144 peak at 18.369 min; Rearrangement peak at 18.594 min

GC/MS TIC: 5-Bromo-UR-144 Lot # 0440444-8



EI Mass Spectrum: 5-Bromo-UR-144 Lot # 0440444-8





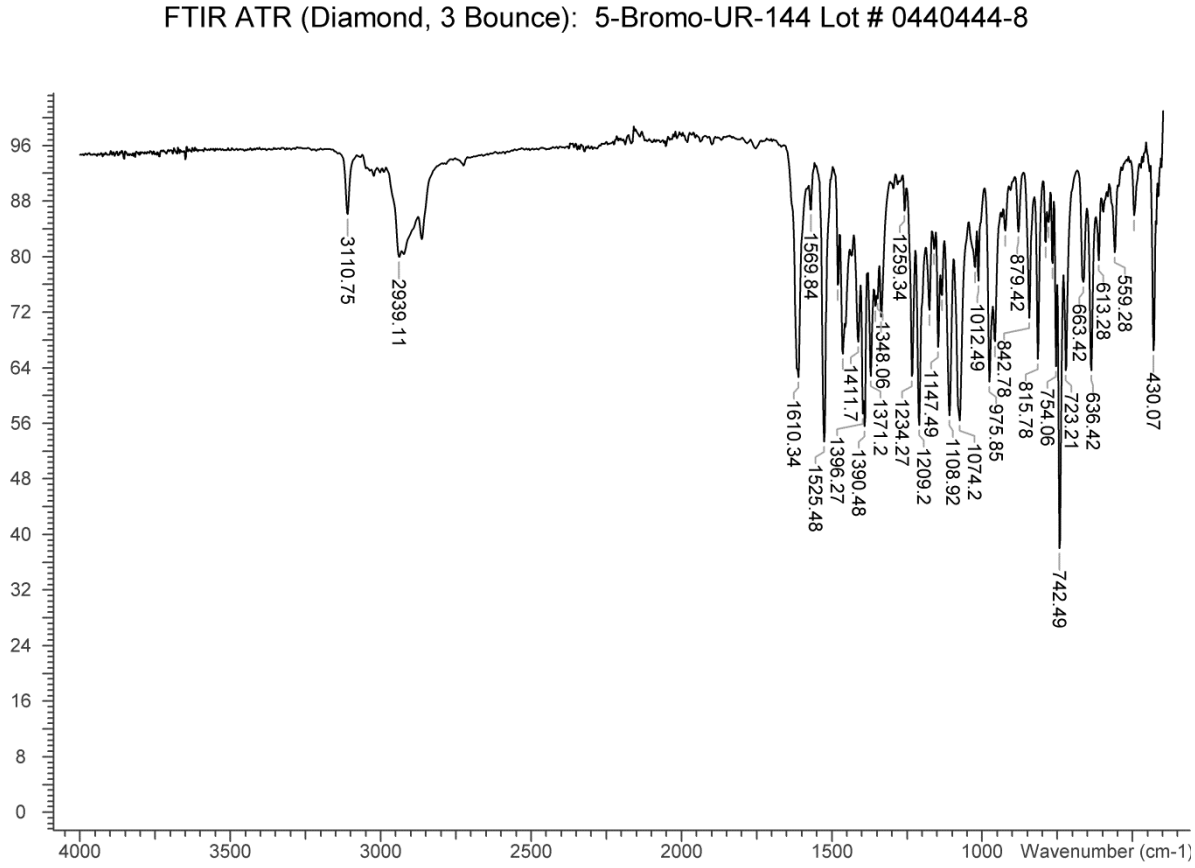
GC/MS Analytical Observation:

The GC/MS TIC of 5-Bromo-UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 18.369 minutes, is 5-Bromo-UR-144 while the minor peak, with a retention time of 18.594 minutes, is a thermally induced rearrangement product of 5-Bromo-UR-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.

The peak at 17.686 minutes is an impurity of 5-Bromo-UR-144.

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-Bromo-UR-144 Lot # 0440444-8