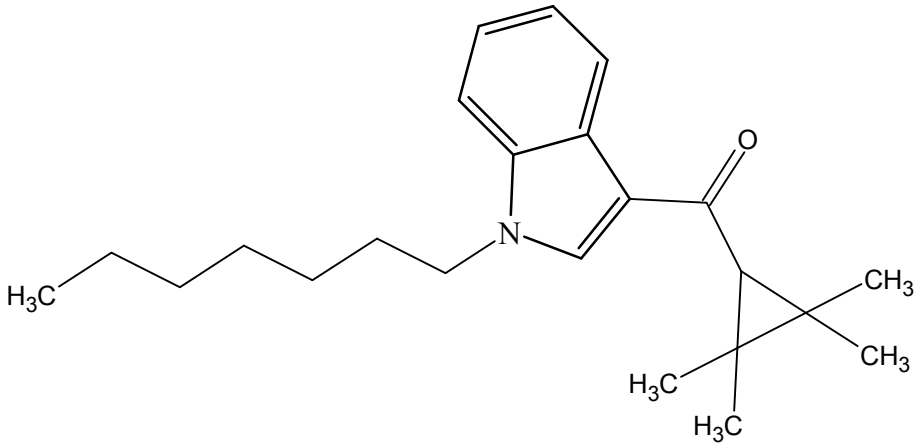
Heptyl-UR-144

Latest Revision: August 30, 2013



1. GENERAL INFORMATION

IUPAC Name: (1-heptyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone

CFR: Not Scheduled (7/2013)

CAS#: Not Available

Synonyms: UR-144 N-heptyl analog

Source: DEA Reference Material Collection

Appearance: White powder

Kovat's Index: Pending

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{23}H_{33}NO$	339	73.7

3. ADDITIONAL RESOURCES

No resources identified as of 8/26/13.

4. QUALITATIVE DATA

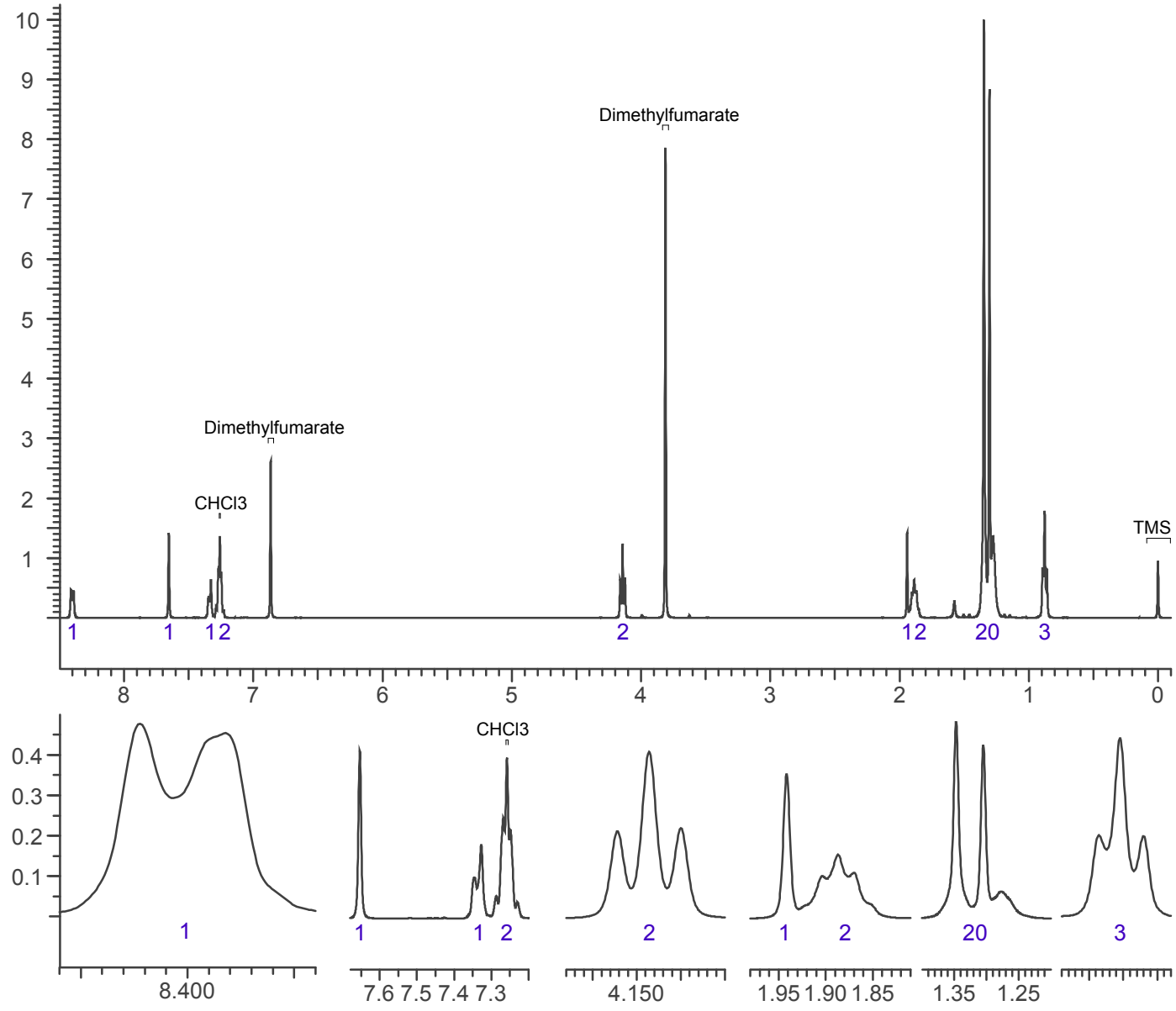
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

Sample Preparation: Dilute analyte to ~10 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and dimethylfumarate 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

^1H NMR: Heptyl-UR-144 Lot # ALB 214-17; $CDCl_3$; 400 MHz

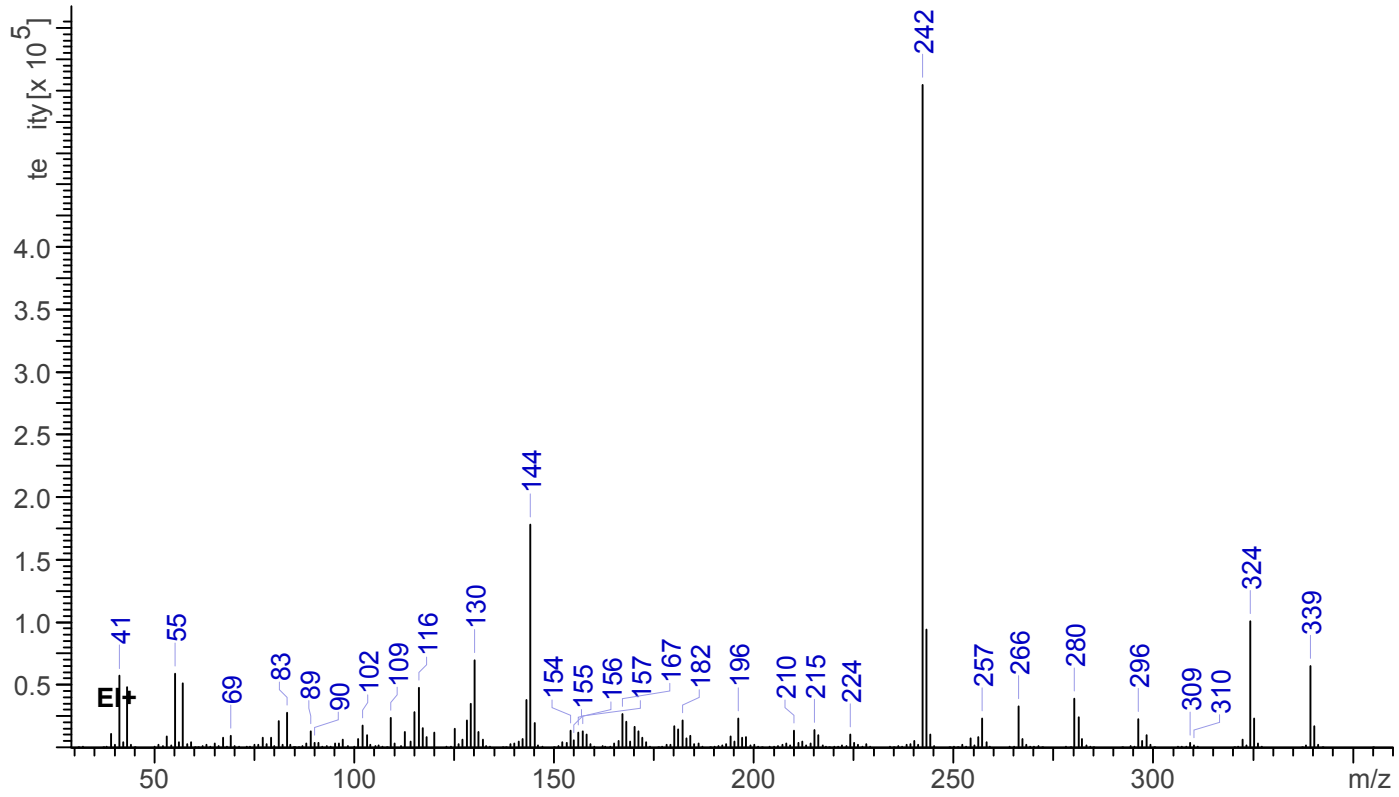


4.2 Gas Chromatography/Mass Spectrometry

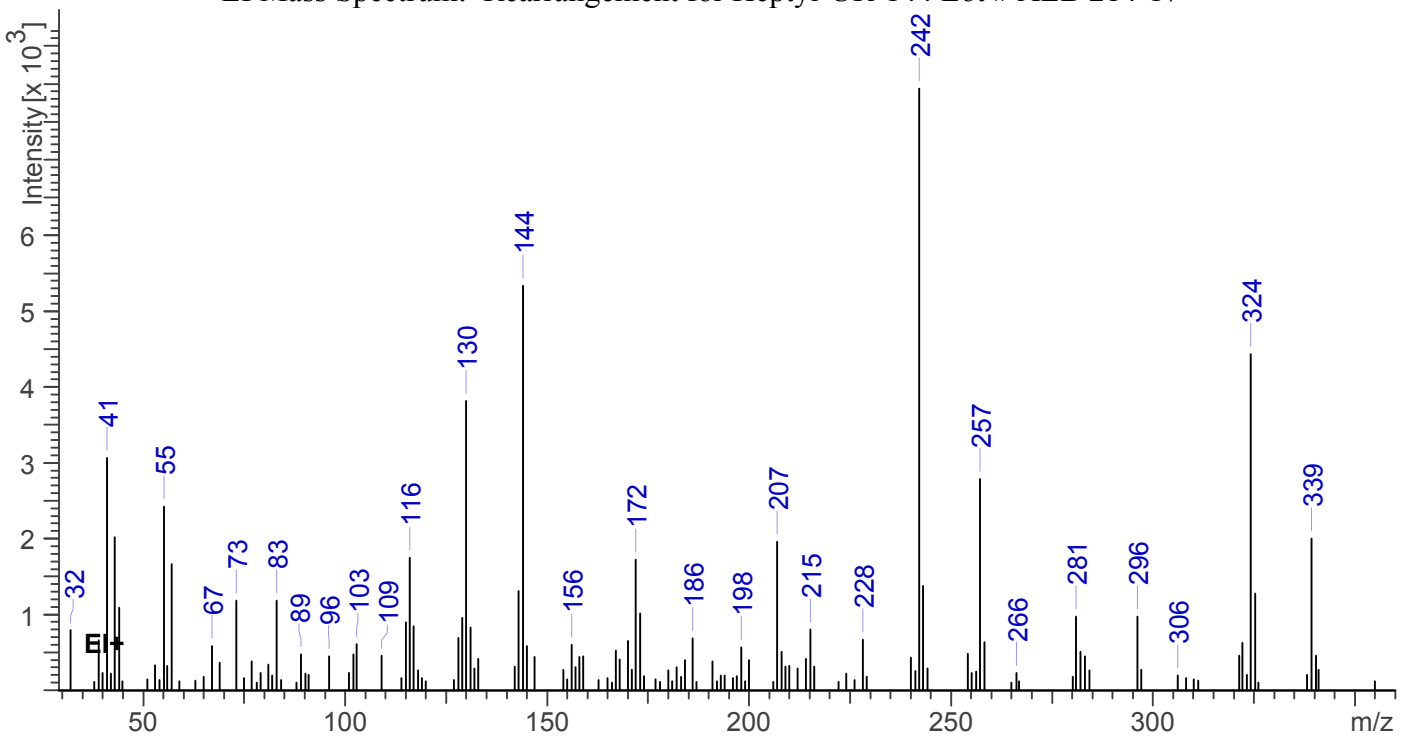
Sample Preparation: Dilute analyte ~1 mg/mL in 9:1 $CHCl_3$/MeOH.

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 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:	Heptyl-UR-144: 16.87 min; Rearrangement: 17.05 min

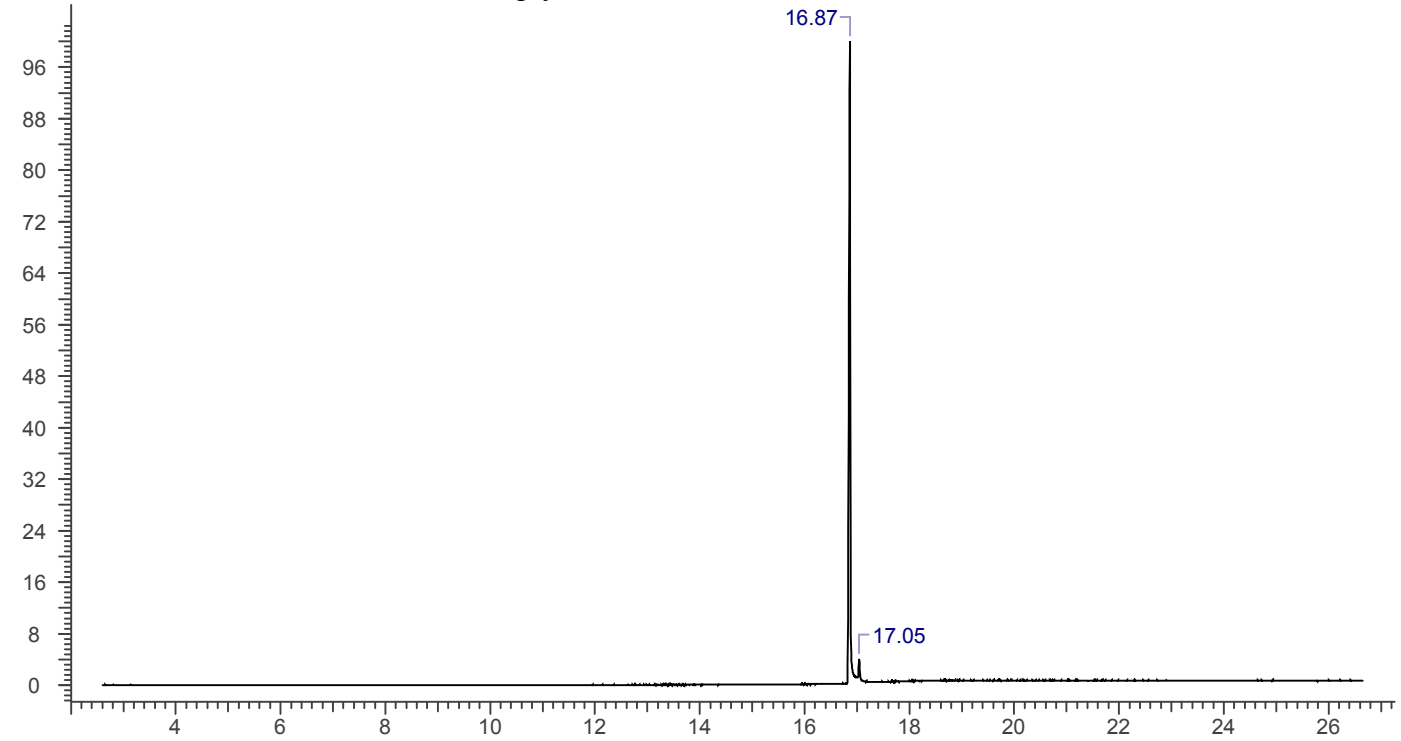
EI Mass Spectrum: Heptyl-UR-144 Lot # ALB 214-17



EI Mass Spectrum: Rearrangement for Heptyl-UR-144 Lot # ALB 214-17



TIC: Heptyl-UR-144 Lot # ALB 214-17



GC/MS Analytical Observation:

The GC/MS TIC of Heptyl-UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 16.87 minutes, is Heptyl-UR-144 while the other peak, with a retention time of 17.05 minutes, is a thermally induced rearrangement product of Heptyl-UR-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.

4.3 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): Heptyl-UR-144 Lot # ALB 214-17