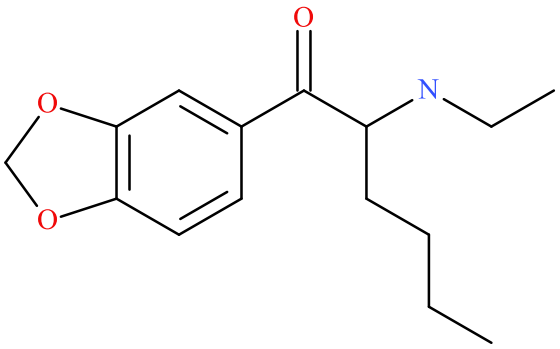
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

N-ethyl Hexylone



Sample Type: **Seized Material**

Latest Revision: **May 18th, 2018**

Date Received: **February 12th, 2018**

Date of Report: **April 19th, 2018**

1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-benzodioxol-5-yl)-2-(ethylamino)hexan-1-one

InChI String: InChI=1S/C15H21NO3/c1-3-5-6-12(16-4-2)15(17)11-7-8-13-14(9-11)19-10-18-13/h7-9,12,16H,3-6,10H2,1-2H3

CFR: Not Scheduled (04/2018)

CAS# Not Available

Synonyms: Not Available

Source: Department of Homeland Security

Appearance: Off-White Solid Material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{15}H_{21}NO_3$	263.33	263	264.1594

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.*

***Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT*

3. BRIEF DESCRIPTION

N-ethyl Hexylone is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include *N*-ethyl pentylone, pentylone, methylone, and butylone. Pentylone, methylone, and butylone are all Schedule I substances in the United States, while *N*-ethyl pentylone is not scheduled in the United States.

4. ADDITIONAL RESOURCES

Koppe, H.; Ludwig, G.; and Zeile, K. Aryl-alpha-Aminoketone Derivatives. CH Boehringer Sohn AG and Co KG, Boehringer Ingelheim GmbH, Assignee. Patent GB1085135A. 08 Apr. 1964.

5. QUALITATIVE DATA

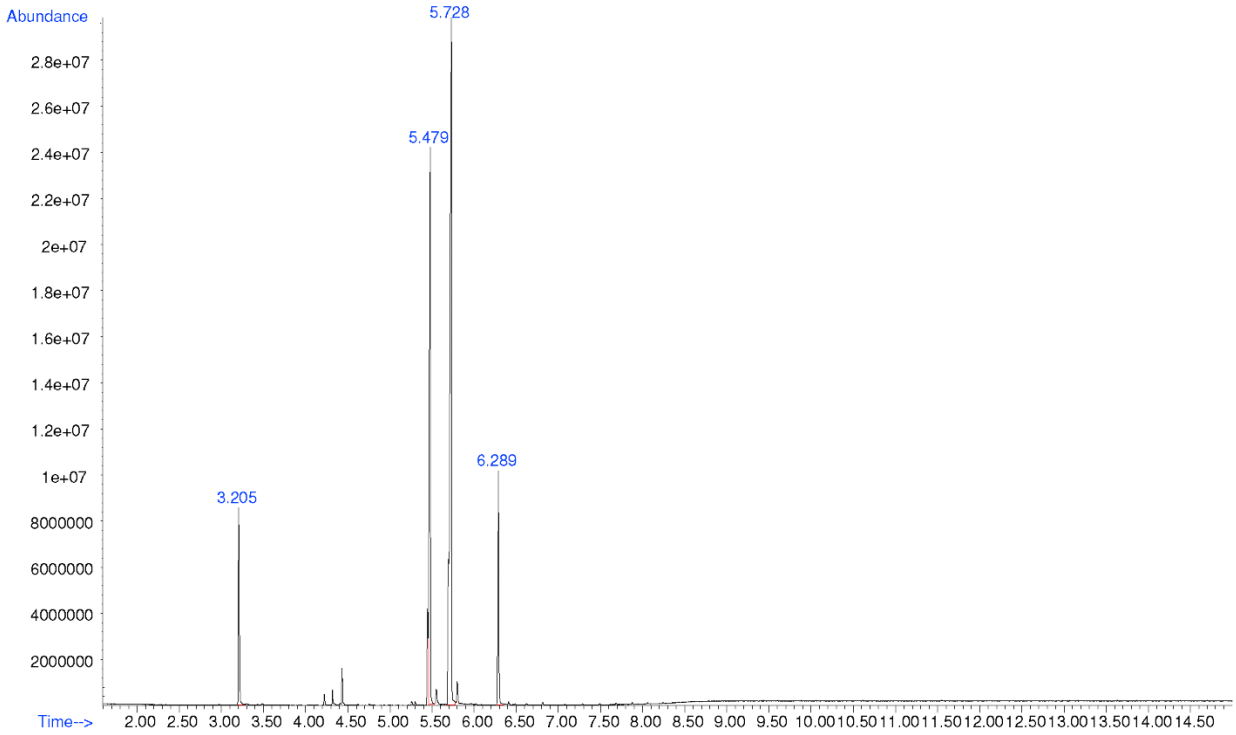
5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z

Threshold: 250

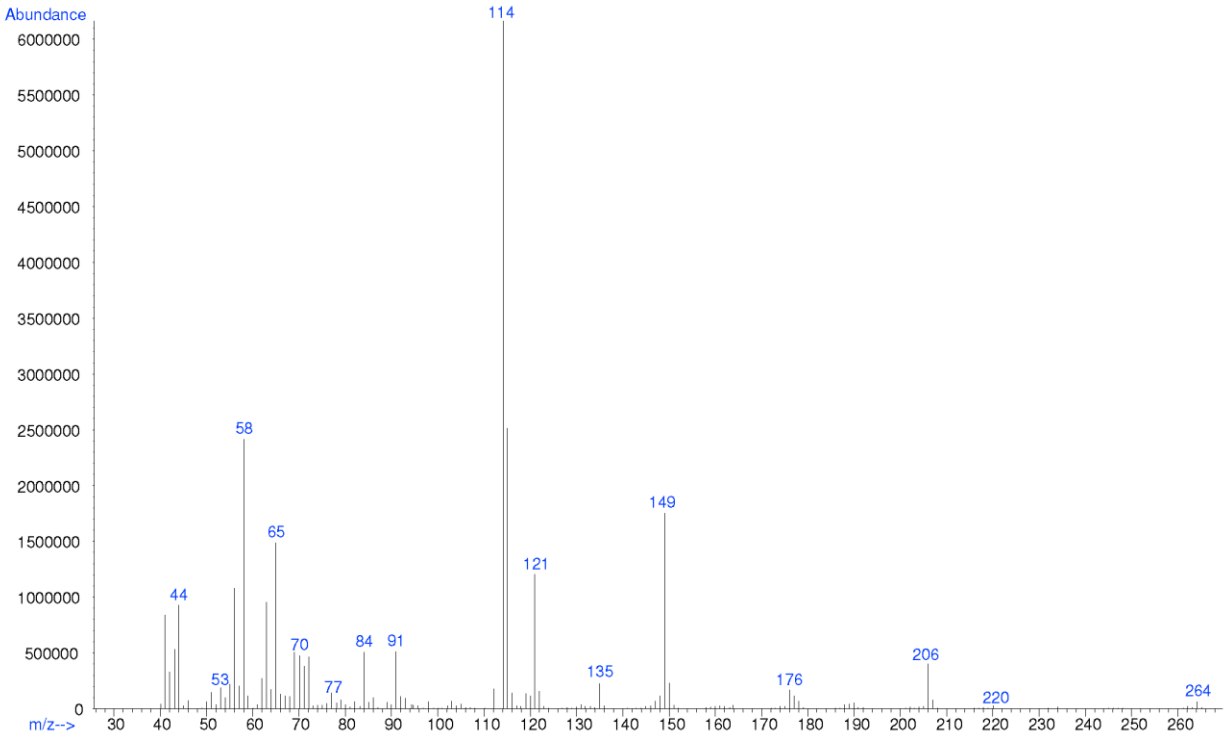
Retention Time: 5.728 min

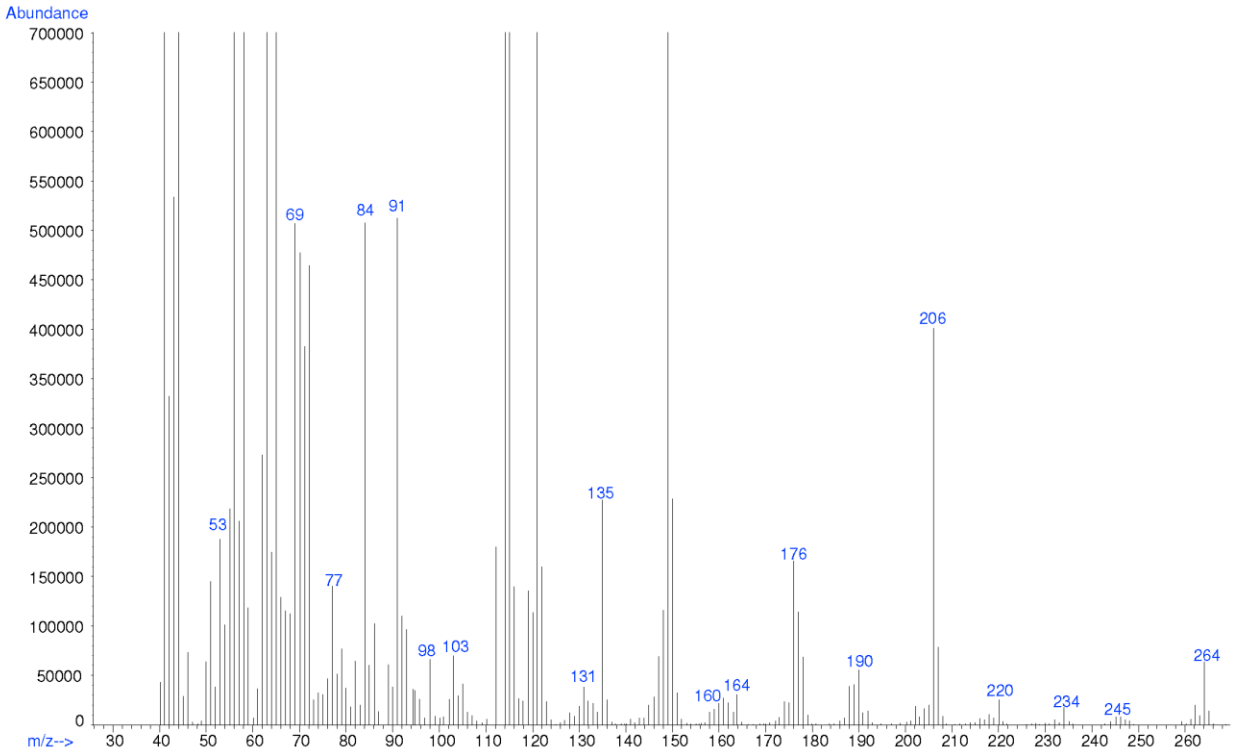
Chromatogram: *N*-ethyl Hexylone



Additional peaks present in chromatogram: internal standard 1 (3.205 min), N-ethyl pentylone (5.479 min), and internal standard 2 (6.289 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-ethyl Hexylone

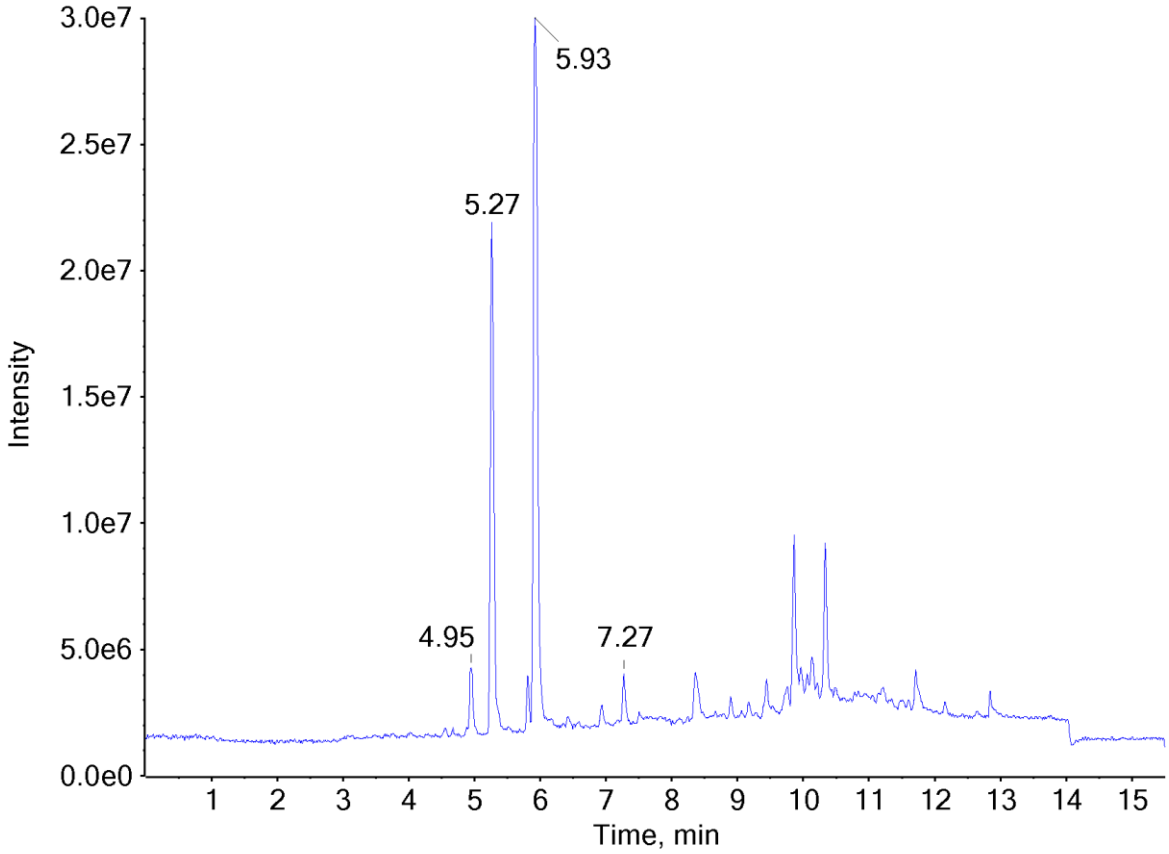




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

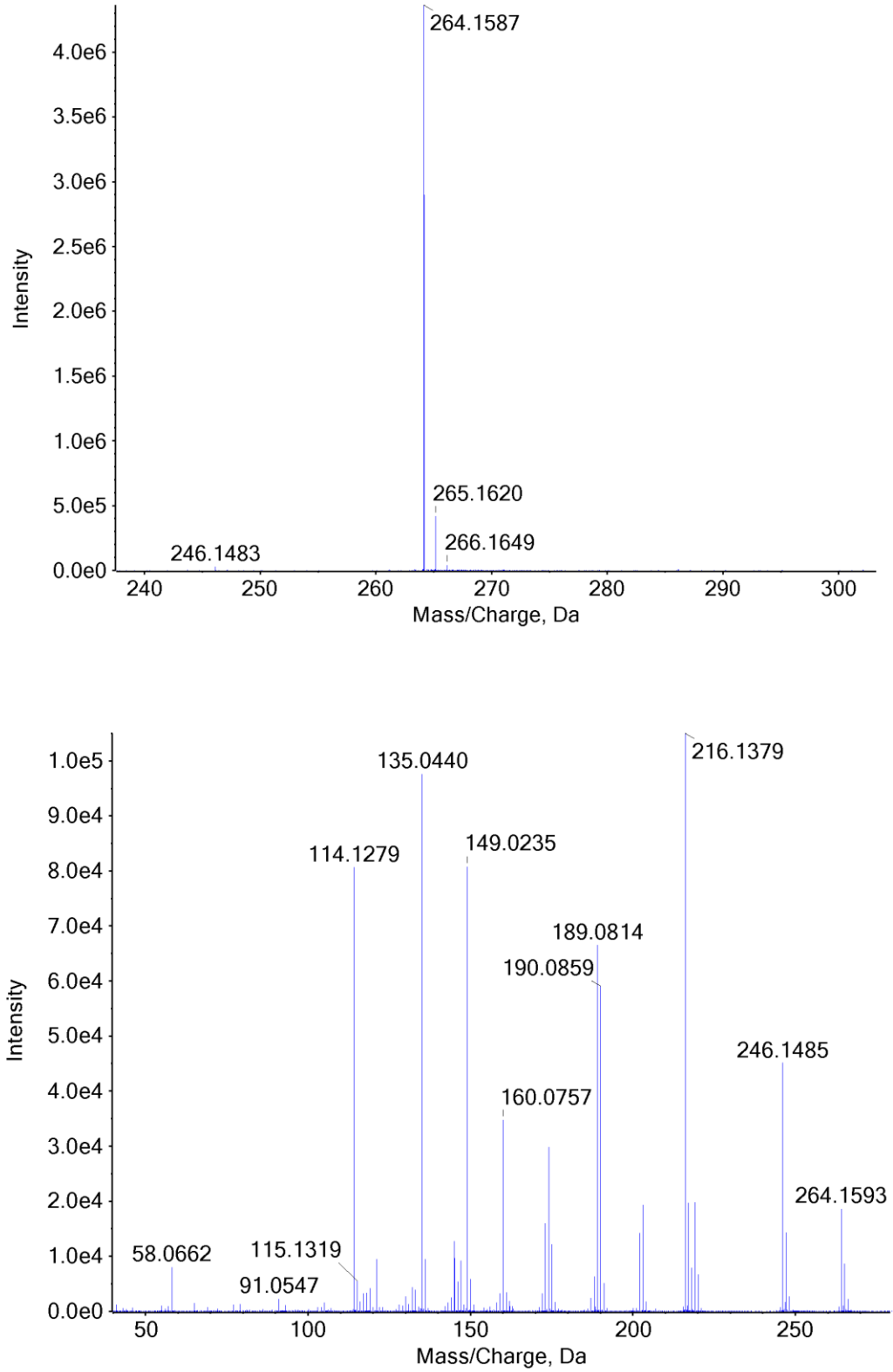
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
Mobile Phase:	A: Ammonium formate (10 mM, pH 3.0)
	B: Methanol/acetonitrile (50:50)
	Flow rate: 0.4 mL/min
Gradient:	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	5.93 min

Chromatogram: *N*-ethyl Hexylone



Additional peaks present in chromatogram: internal standard 1 (4.95 min), N-ethyl pentylone (5.27 min), and internal standard 2 (7.27 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: *N*-ethyl Hexylone



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in $CDCl_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

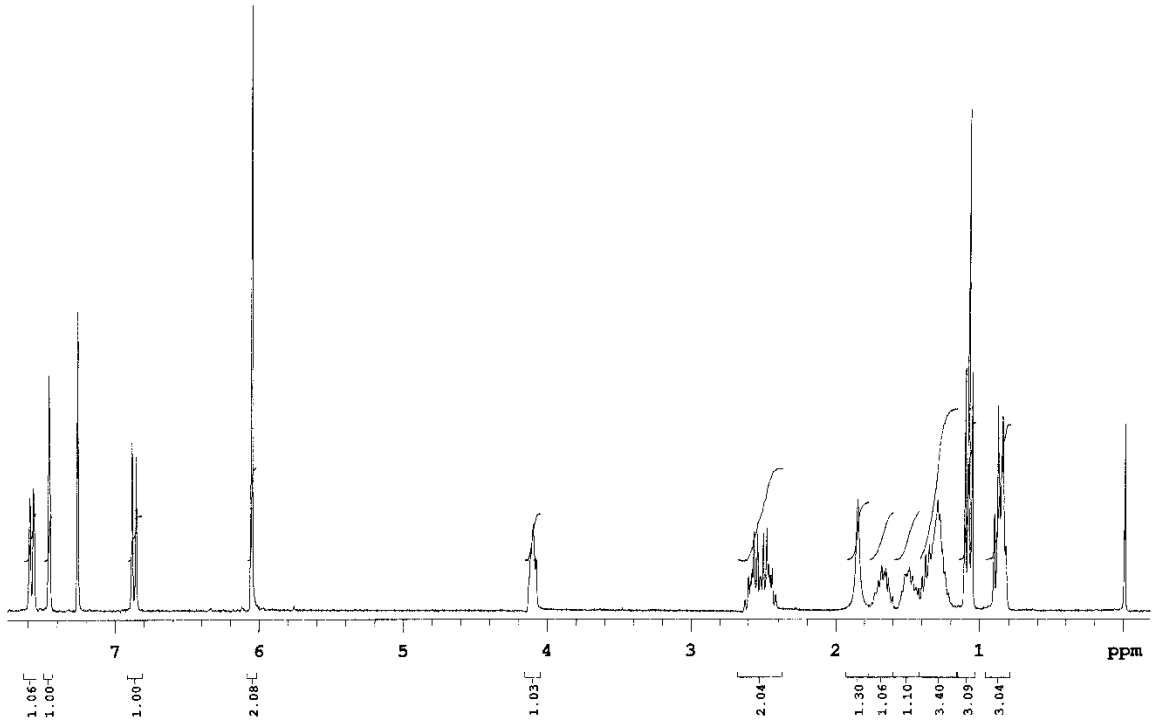
Parameters: Pulse Sequence: Proton

Solvent: $CDCl_3$

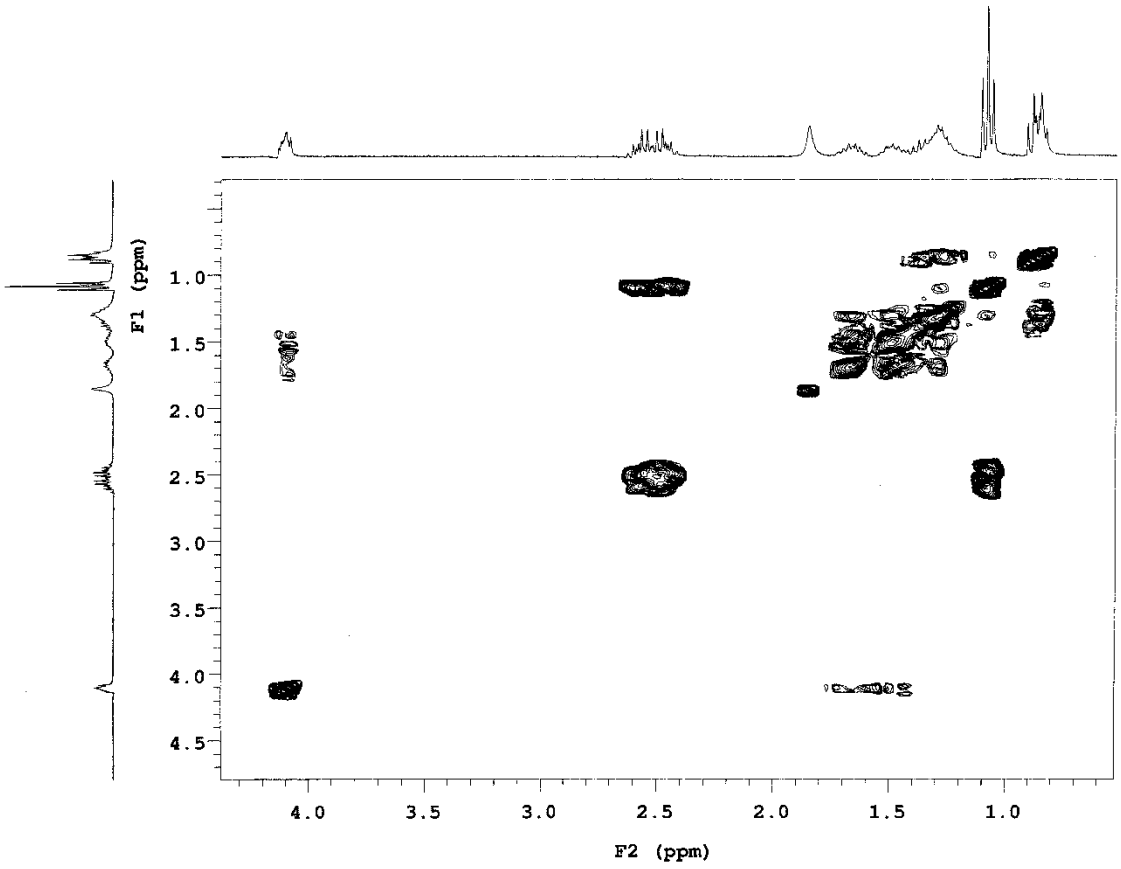
Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

^{1}H NMR: *N*-ethyl Hexylone



gCOSY: *N*-ethyl Hexylone



6. REVISION HISTORY

Date	Revision
05/18/2018	Added "Sample Type: Seized Material" to Page 1.
05/18/2018	Added "Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT" to Page 1 footer.