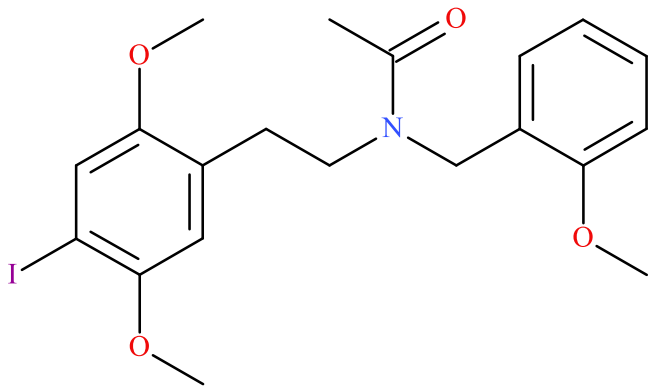
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

N-Acetyl 25I-NBOMe

Sample Type: **Seized Material**



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

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

Date of Report: **February 27th, 2018**

1. GENERAL INFORMATION

IUPAC Name:	N-[2-(4-iodo-2,5-dimethoxy-phenyl)ethyl]-N-[(2-methoxyphenyl) methyl]acetamide
InChI String:	InChI=1S/C20H24INO4/c1-14(23)22(13-16-7-5-6-8-18(16)24-2)10-9-15-11-20(26-4)17(21)12-19(15)25-3/h5-8,11-12H,9-10,13H2,1-4H3
CFR:	Not Scheduled (02/2018)
CAS#	Not available
Synonyms:	Acetylated 25I-NBOMe, 25I-NBOME AC
Source:	Department of Homeland Security
Appearance:	Off-white solid material

***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*

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{20}H_{24}INO_4$	469.3	469	470.0823

3. BRIEF DESCRIPTION

N-Acetyl-25I-NBOMe is classified as a phenethylamine with proposed hallucinogenic properties based on its derivation from 25I-NBOMe. Phenethylamines are modified based on the structure of phenethylamine, comprised of a phenyl ring, two carbon chain, and amine moiety. Phenethylamines have been reported to cause stimulant and hallucinogenic effects, dependent on their structure and modifications. Phenethylamines have been associated with adverse events, including deaths, as described in the literature. Structurally similar compounds include 2C-I and 25I-NBOMe (Cimbi-27). 2C-I and 25I-NBOMe are Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

https://www.chemograph.de/dd2017/dd2017-18634-916259.html

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)

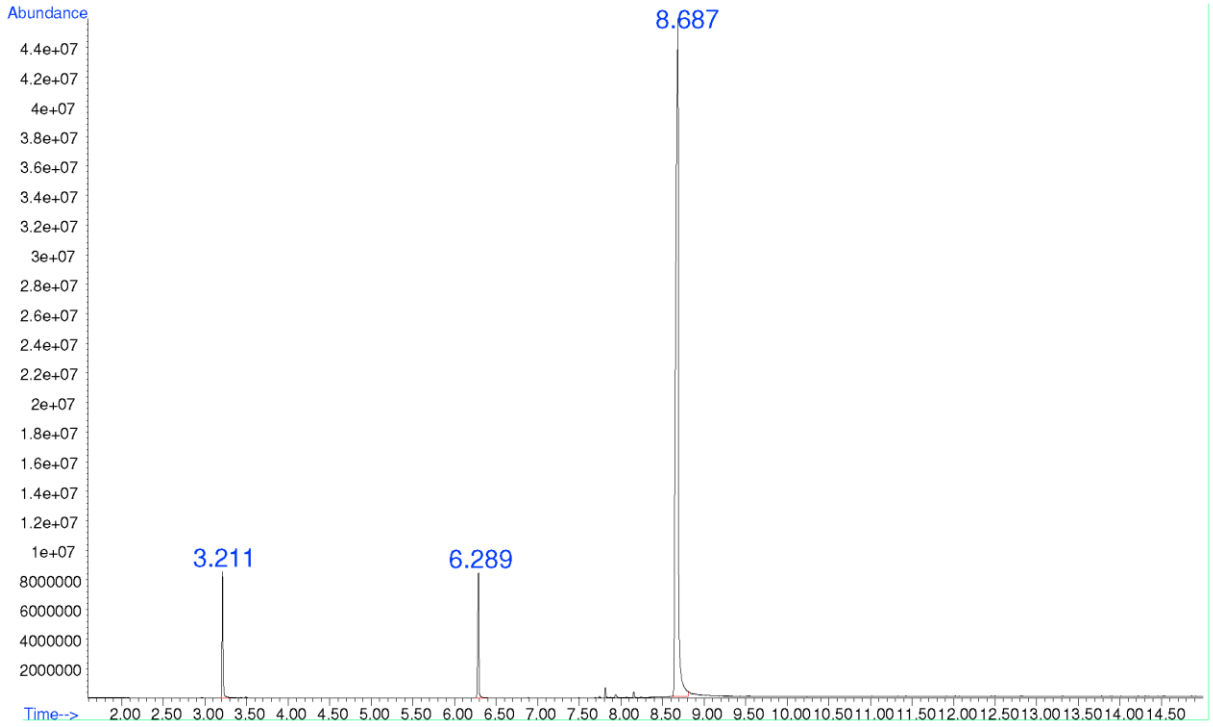
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

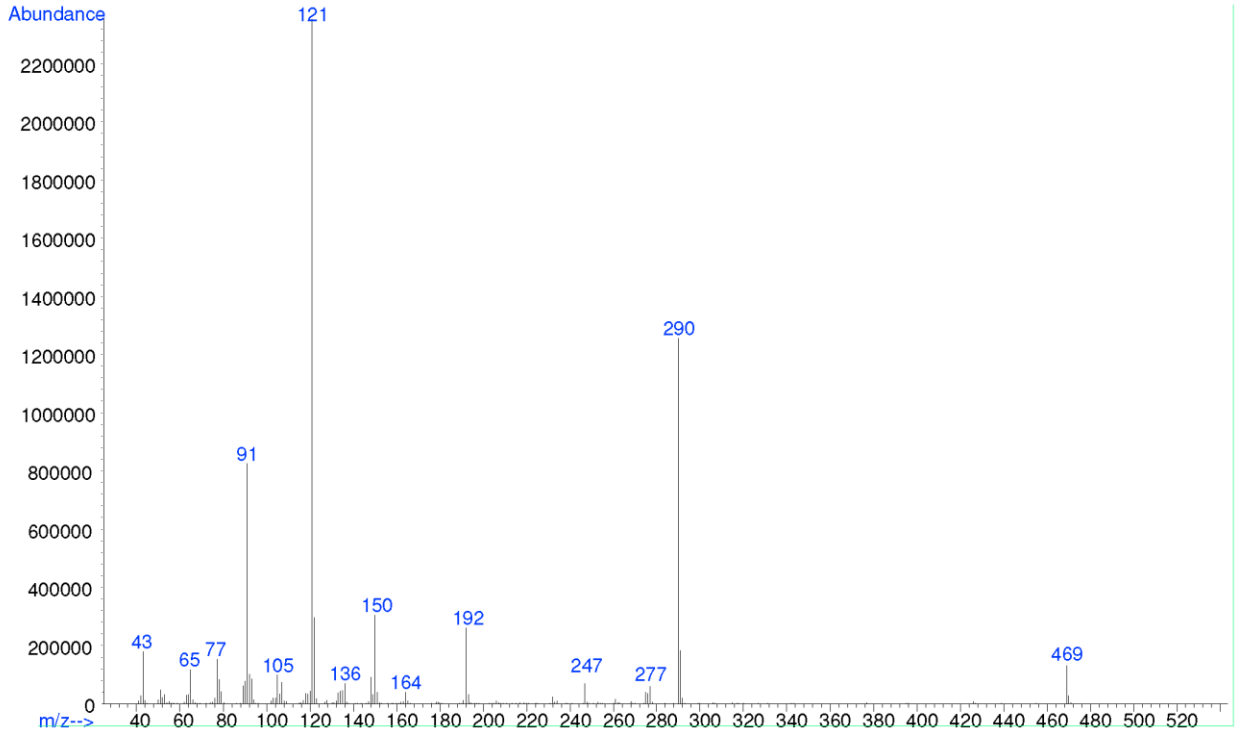
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.687 min

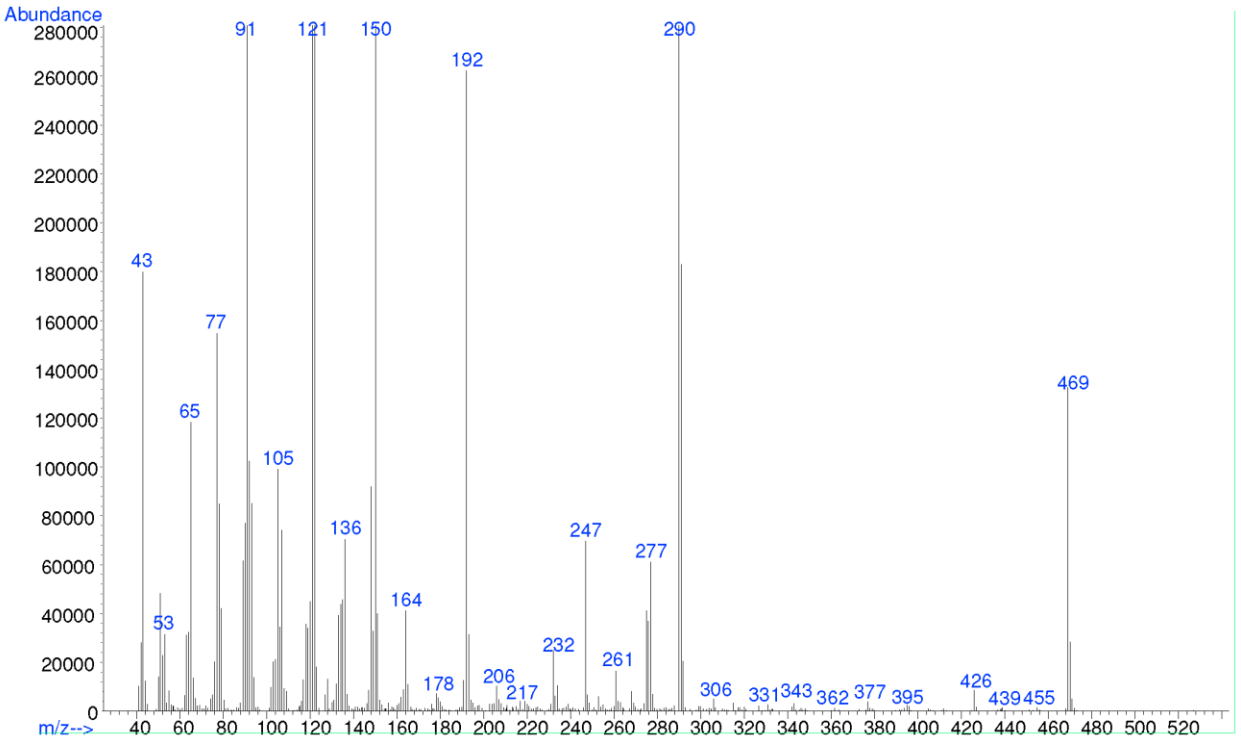
Chromatogram: *N*-Acetyl-25I-NBOMe



Additional peaks present in chromatogram: internal standard 1 (3.211 min), internal standard 2 (6.289 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-Acetyl-25I-NBOMe

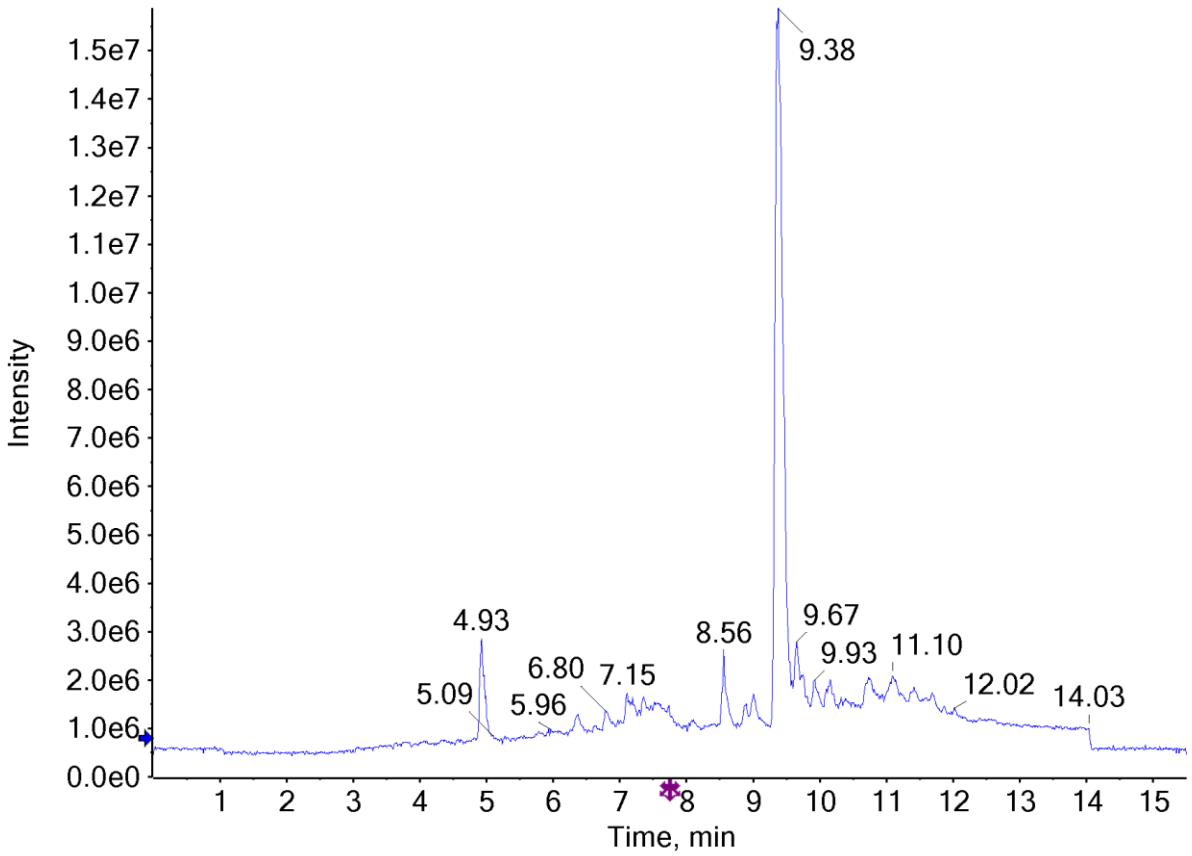




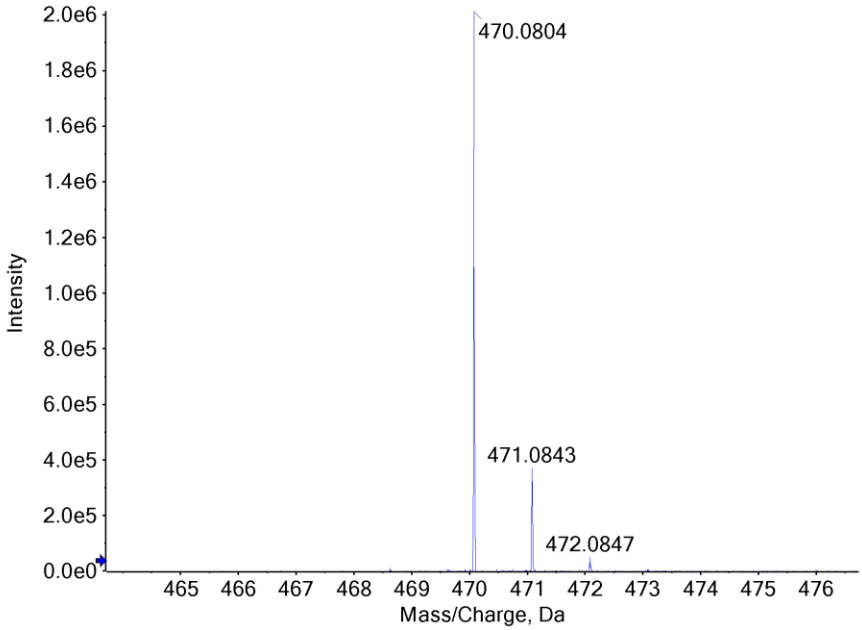
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

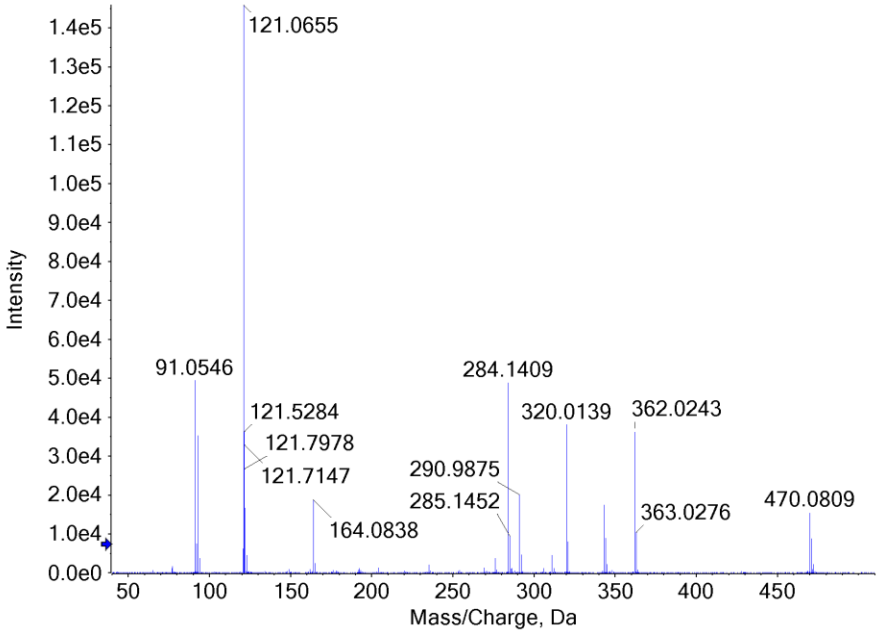
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	9.38 min

Chromatogram: *N*-Acetyl-25I-NBOMe



TOF MS (Top) and MS/MS (Bottom) Spectra: *N*-Acetyl-25I-NBOMe





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

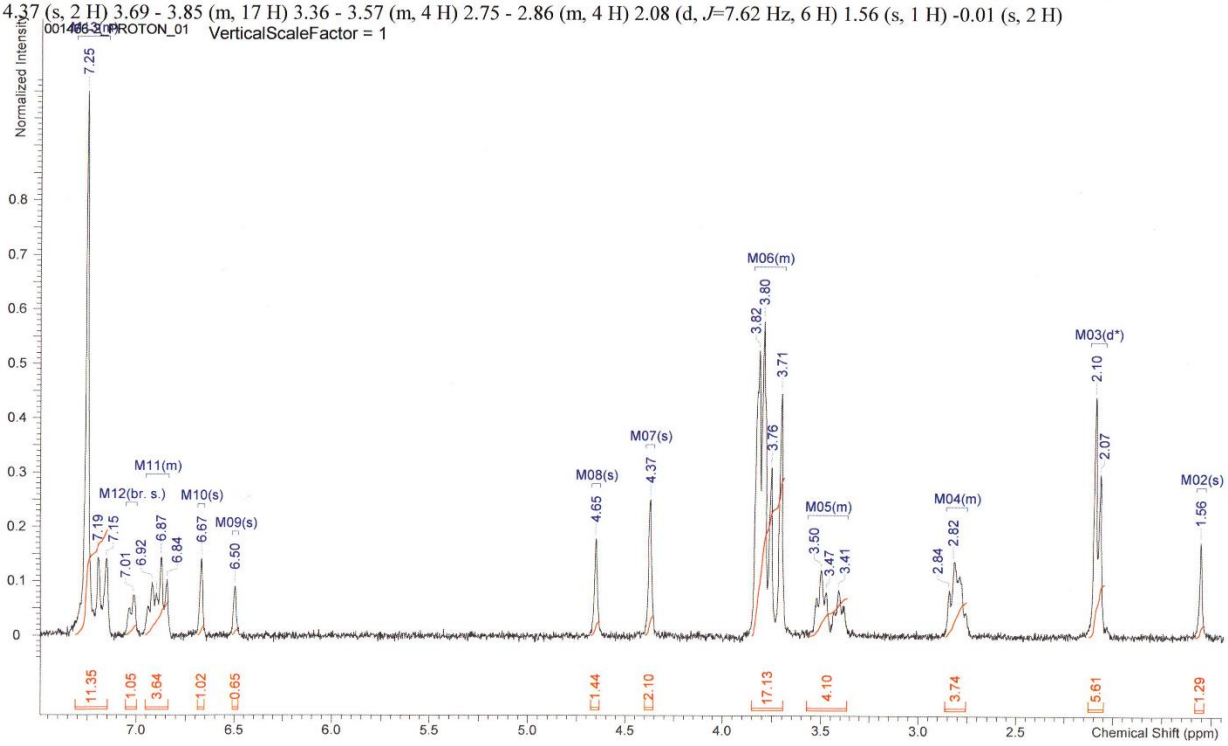
Solvent: $CDCl_3$

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*-Acetyl-25I-NBOMe

^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm 7.15 - 7.31 (m, 11 H) 7.01 (br. s., 1 H) 6.83 - 6.95 (m, 4 H) 6.67 (s, 1 H) 6.50 (s, 1 H) 4.65 (s, 1 H) 4.37 (s, 2 H) 3.69 - 3.85 (m, 17 H) 3.36 - 3.57 (m, 4 H) 2.75 - 2.86 (m, 4 H) 2.08 (d, *J*=7.62 Hz, 6 H) 1.56 (s, 1 H) -0.01 (s, 2 H)



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.