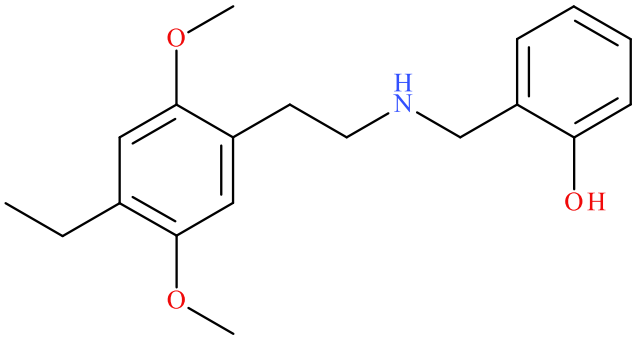
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

25E-NBOH

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: 2-[[2-(4-ethyl-2,5-dimethoxy-phenyl)ethylamino]methyl]phenol

InChI String: InChI=1S/C19H25NO3/c1-4-14-11-19(23-3)15(12-18(14)22-2)9-10-20-13-16-7-5-6-8-17(16)21/h5-8,11-12,20-21H,4,9-10,13H2,1-3H3

CFR: Not Scheduled (02/2018)

CAS# Not available

Synonyms: NBOH-2C-E

Source: Department of Homeland Security

Appearance: 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	$C_{19}H_{25}NO_3$	315.4	315	316.1907

***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

25E-NBOH is classified as a phenethylamine with proposed hallucinogenic properties based on its derivation from 2C-E and structural similarity to 25E-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-E, 25E-NBOME, and 25I-NBOH (Cimbi-27). 2C-E is a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES

Hansen, M., Phonekeo, K., Paine, J.S., Leth-Petersen, S., Begtrup, M., Bräuner-Osborne, H., et al. (2014) Synthesis and Structure–Activity Relationships of N -Benzyl Phenethylamines as 5-HT 2A/2C Agonists. ACS Chemical Neuroscience, **5**, 243–249.

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/25E-NBOH-ID-1901-18_report.pdf

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

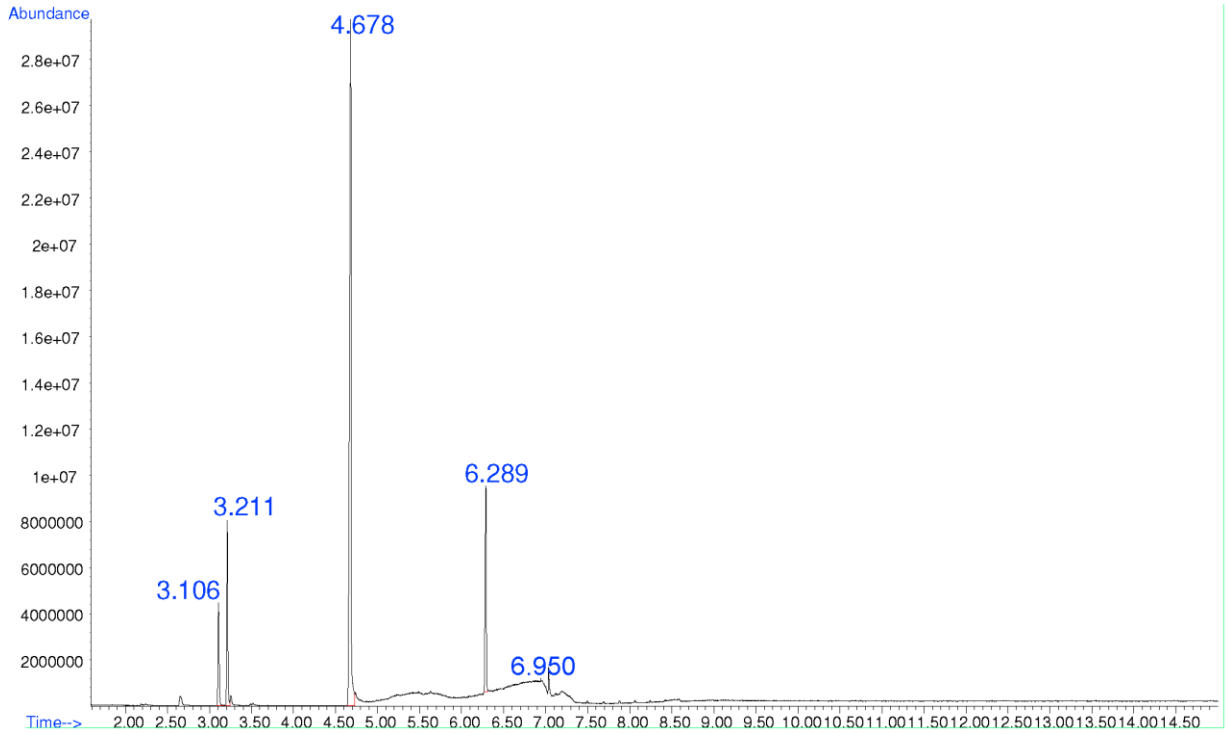
Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

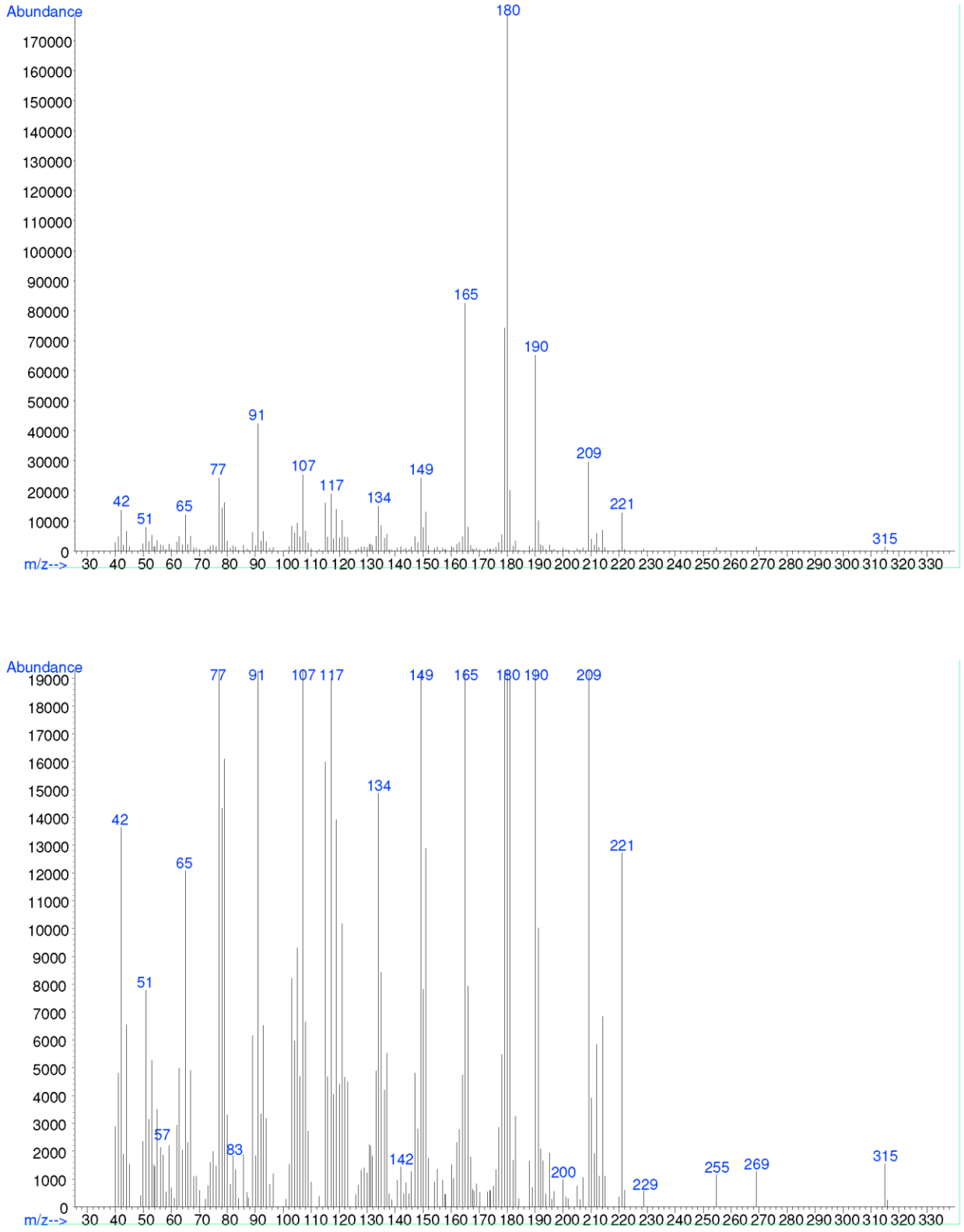
Retention Time: approx. 6.950 min

Chromatogram: 25E-NBOH



Additional peaks present in chromatogram: not a controlled substance (3.106 min), internal standard 1 (3.211 min), 2C-E (4.678 min), internal standard 2 (6.289 min)

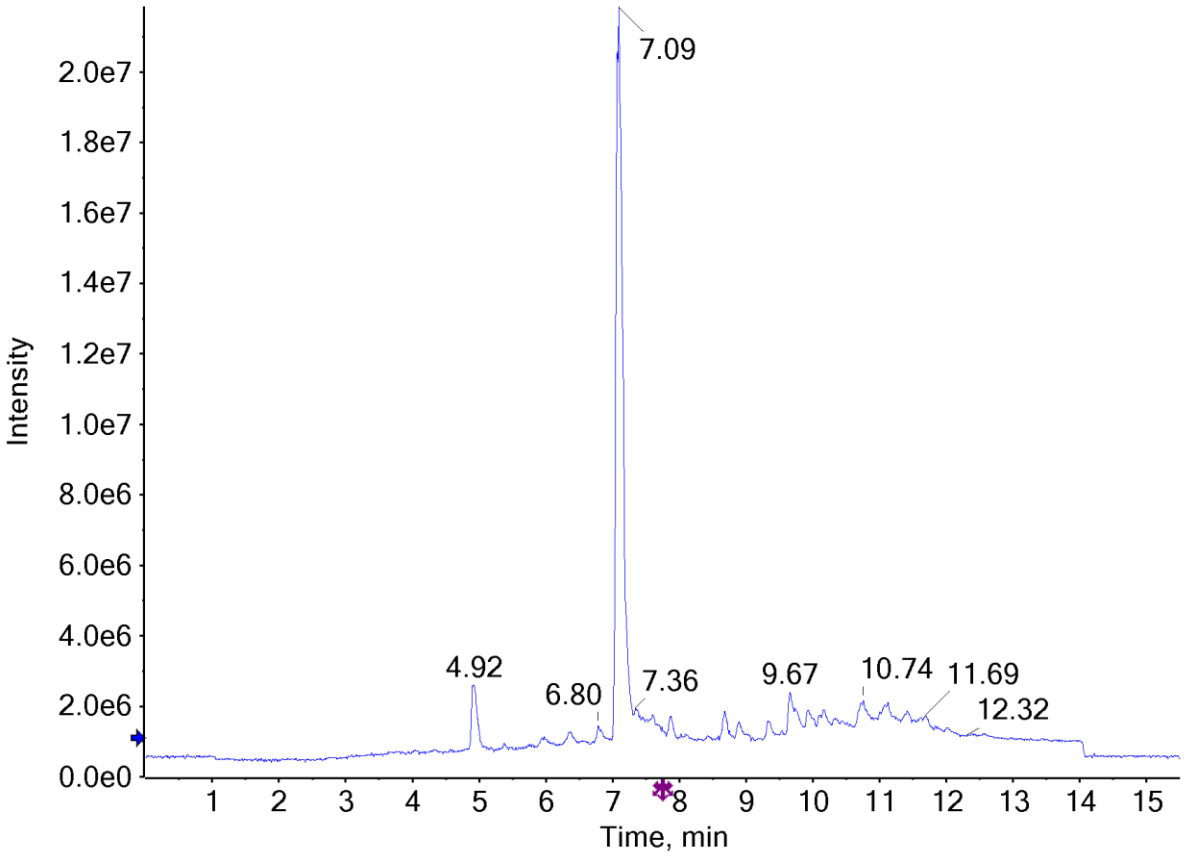
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 25E-NBOH



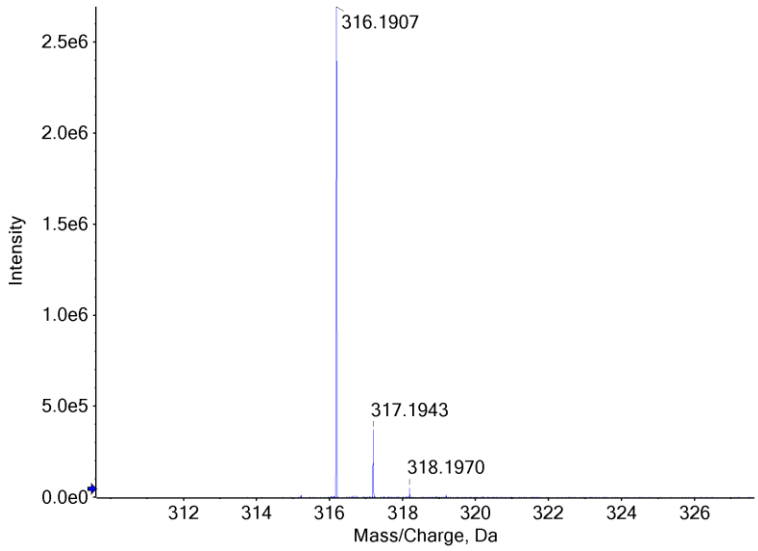
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

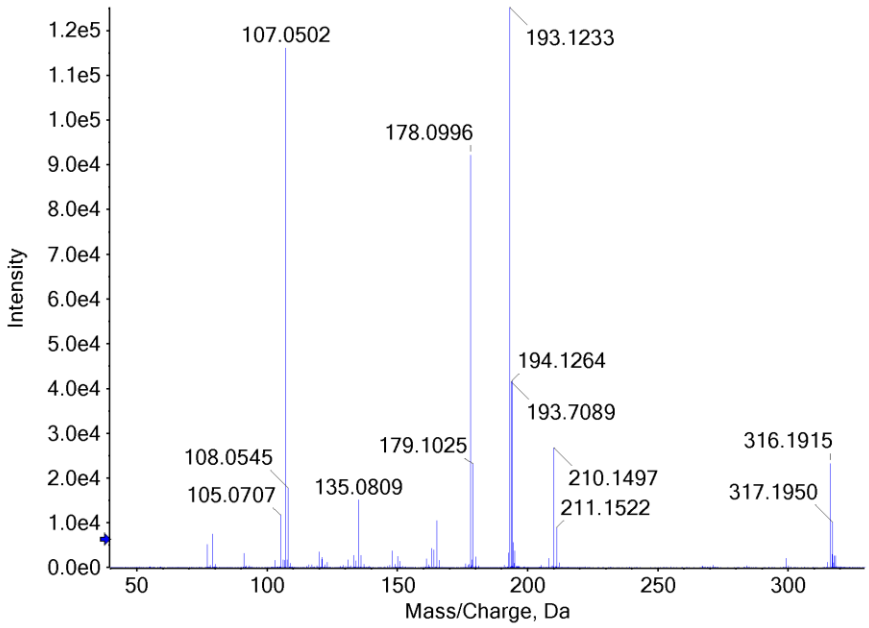
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	7.09 min

Chromatogram: 25E-NBOH



TOF MS (Top) and MS/MS (Bottom) Spectra: 25E-NBOH





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

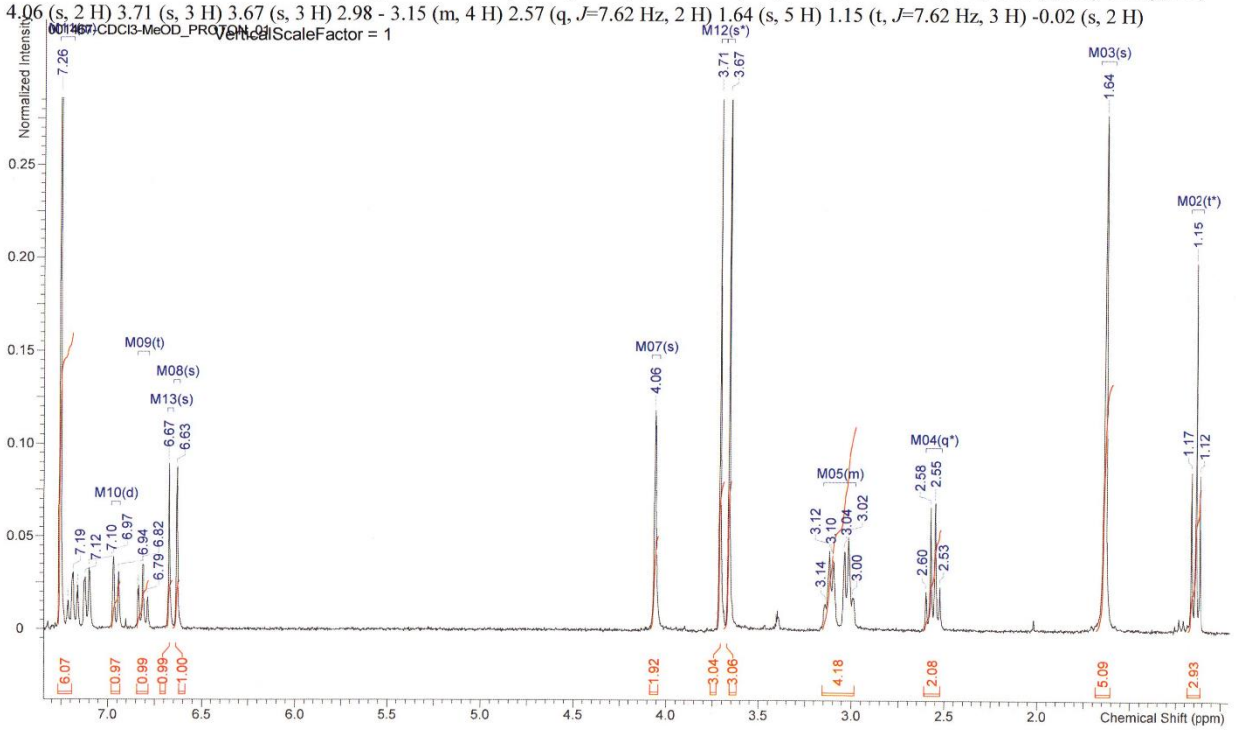
Solvent: $CDCl_3$

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: 25E-NBOH

^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm 7.19 - 7.26 (m, 6 H) 6.96 (d, *J*=7.62 Hz, 1 H) 6.82 (t, *J*=7.25 Hz, 1 H) 6.67 (s, 1 H) 6.63 (s, 1 H) 4.06 (s, 2 H) 3.71 (s, 3 H) 3.67 (s, 3 H) 2.98 - 3.15 (m, 4 H) 2.57 (q, *J*=7.62 Hz, 2 H) 1.64 (s, 5 H) 1.15 (t, *J*=7.62 Hz, 3 H) -0.02 (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.