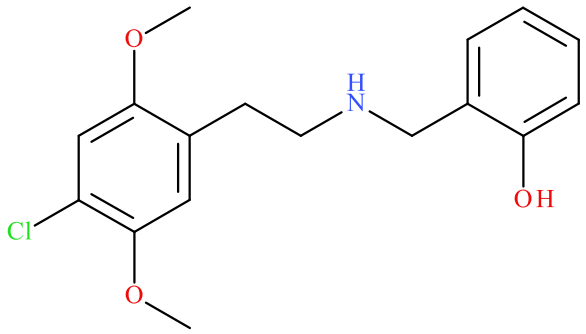
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

25C-NBOH



Sample Type: **Seized Material**

Latest Revision: **March 11, 2019**

Date Received: **August 17, 2018**

Date of Report: **March 11, 2019**

1. GENERAL INFORMATION

IUPAC Name: 2-[[2-(4-chloro-2,5-dimethoxy-phenyl)ethylamino]methyl]phenol

InChI String: InChI=1S/C17H20ClNO3/c1-21-16-10-14(18)17(22-2)9-12(16)7-8-19-11-13-5-3-4-6-15(13)20/h3-6,9-10,19-20H,7-8,11H2,1-2H3

CFR: Not Scheduled (10/2018)

CAS# 1539266-20-0

Synonyms: 2C-C-NBOH, NBOH-2CC

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	$C_{17}H_{20}ClNO_3$	321.8	321	322.1204

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material.*

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

3. BRIEF DESCRIPTION

25C-NBOH is classified as a phenethylamine with proposed hallucinogenic properties based on its derivation from 2C-C and structural similarity to 25C-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. 2C-C and 25C-NBOMe are Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/14815

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/25C-NBOH-ID-1217-15-report_final.pdf

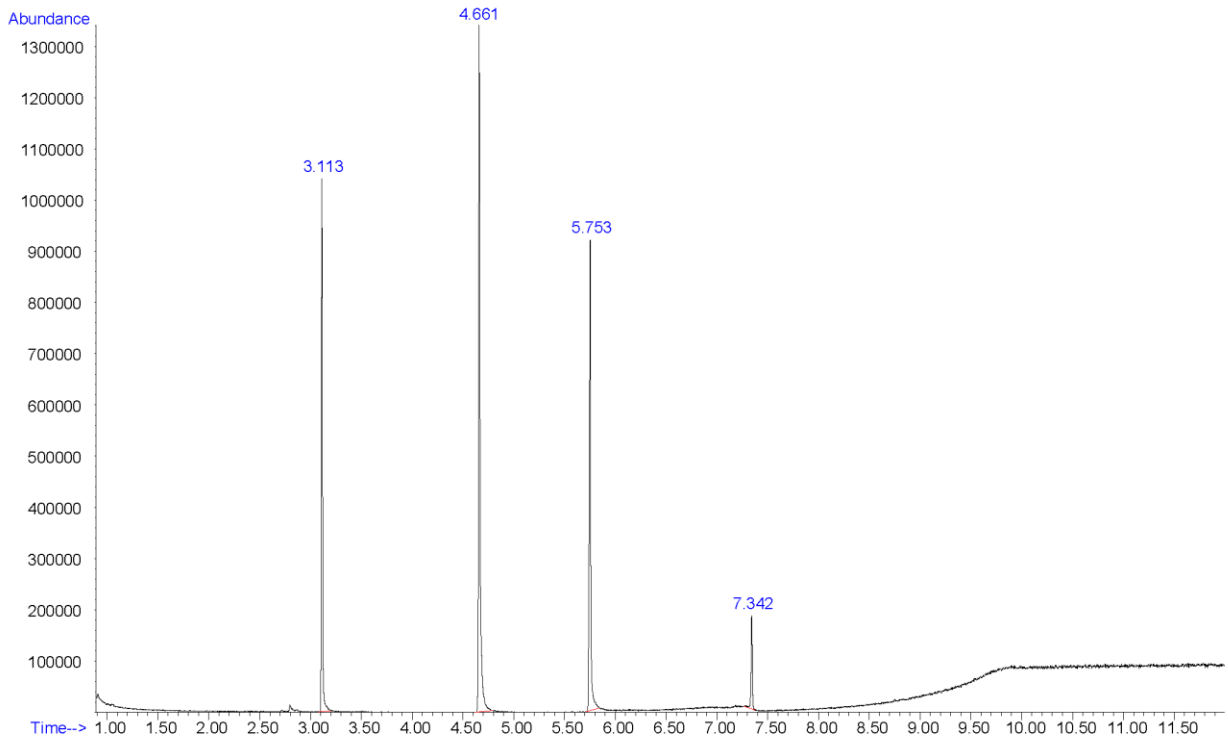
5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/base extraction (25C-NBOH)
	Derivatization required due to thermal instability of 25C-NBOH: Add 50 µL acetic anhydride to extract vial, incubate at room temperature for 30 mins, add 50 µL concentrated NH_4OH, vortex, allow mixture to settle, re-analyze (25C-NBOH derivatives)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: 1.46 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C

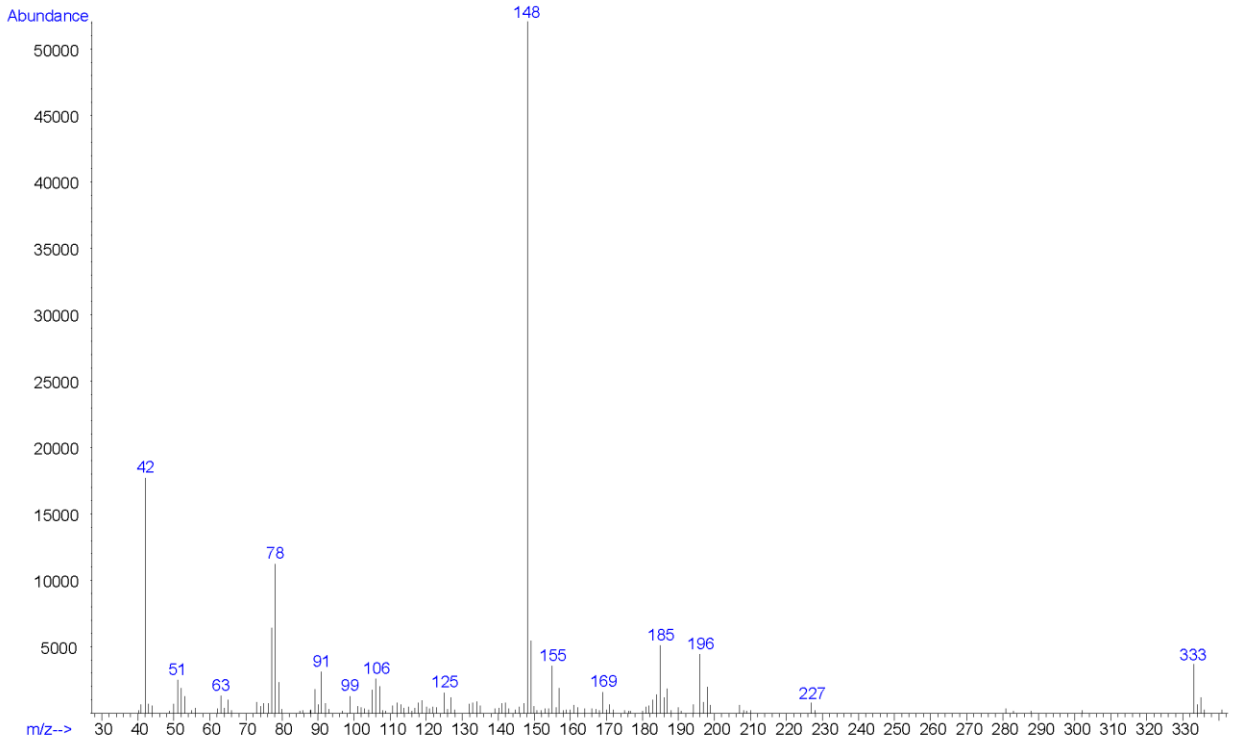
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	25C-NBOH suspected formyl artifact: approx. 7.342 min
	25C-NBOH monoacetyl- derivative: 8.118 min
	25C-NBOH diacetyl- derivative: 8.171 min
Standard Comparison:	Reference material for 25C-NBOH (Batch: 0464724-22) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 25C-NBOH, based on retention time and mass spectral data for acetylated derivatives (25C-NBOH monoacetyl- derivative: 8.087 min; 25C-NBOH diacetyl- derivative: 8.087 min). Analysis of 25C-NBOH underivatized resulted in breakdown to 2C-C artifact; therefore, no retention time and mass spectral data was available for parent 25C-NBOH from the standard. (https://www.caymanchem.com/product/14815)

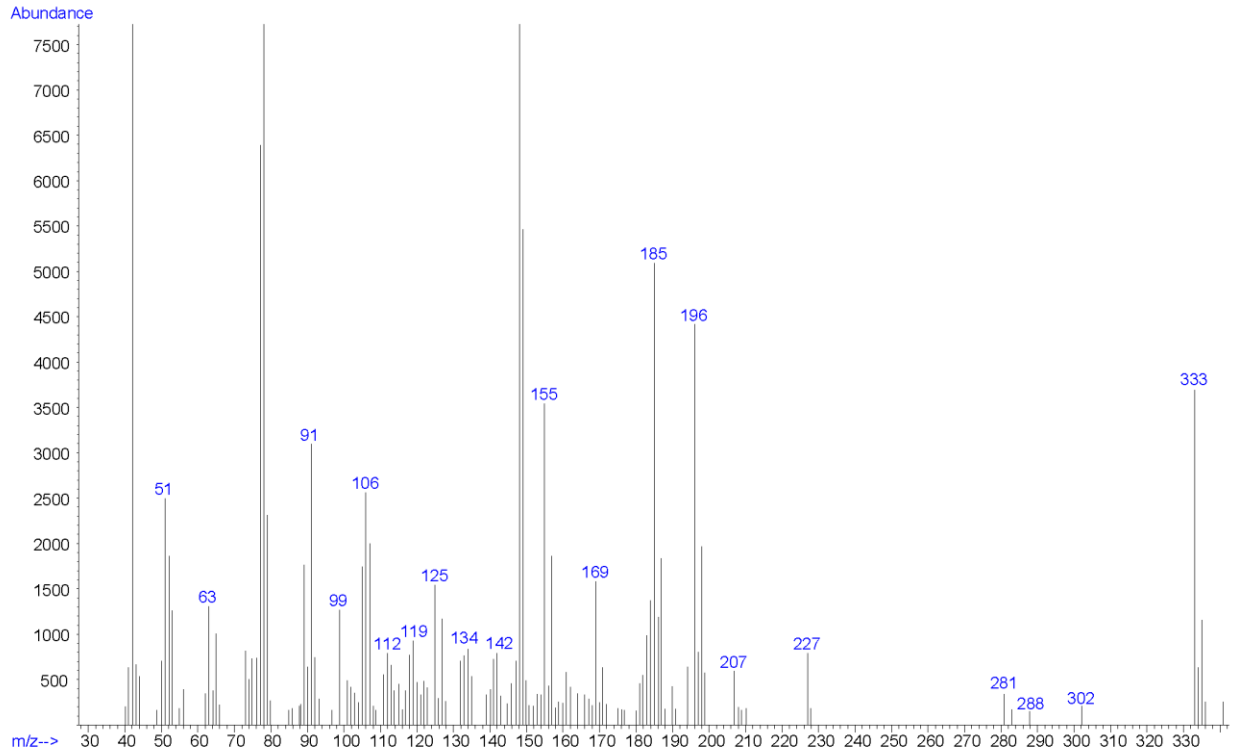
Chromatogram: 25C-NBOH (Seized Exhibit - Underivatized)



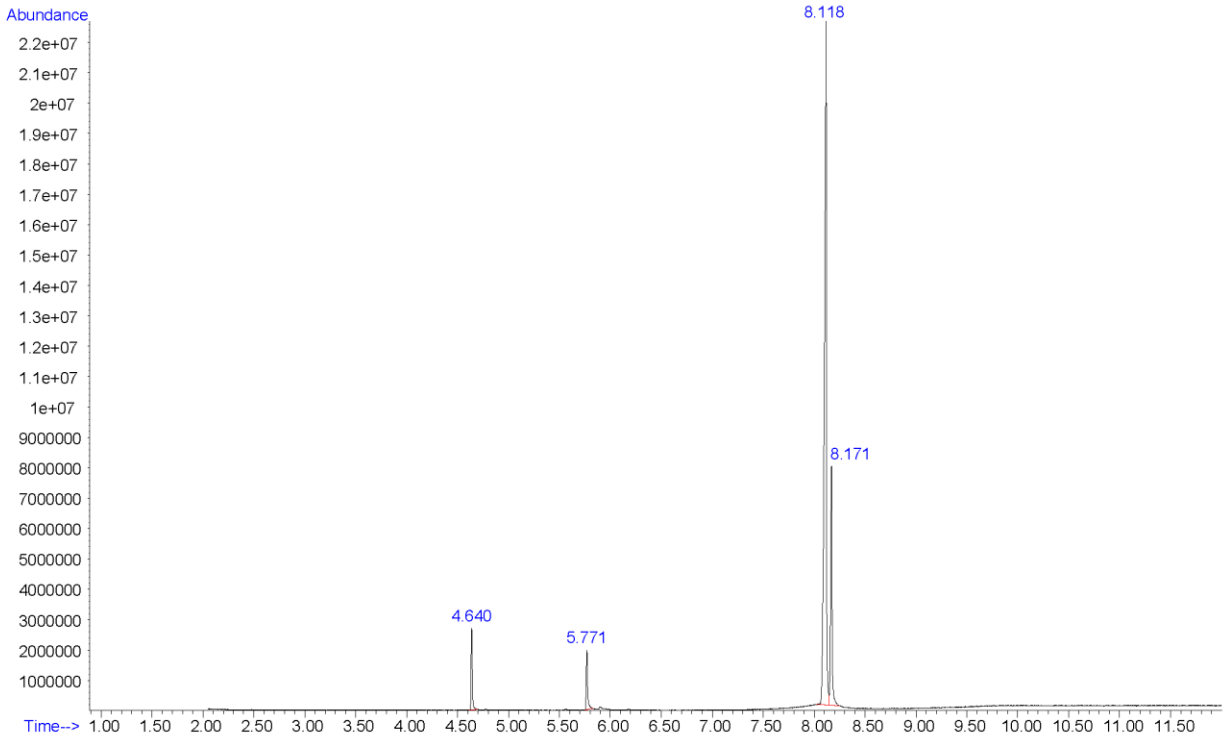
Additional peaks present in chromatogram: internal standard (3.113 min), 2C-C [thermal degradation product] (4.661 min), internal standard (5.753 min), 25C-NBOH suspected formyl artifact (approx. 7.342)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 25C-NBOH Suspected Formyl Artifact



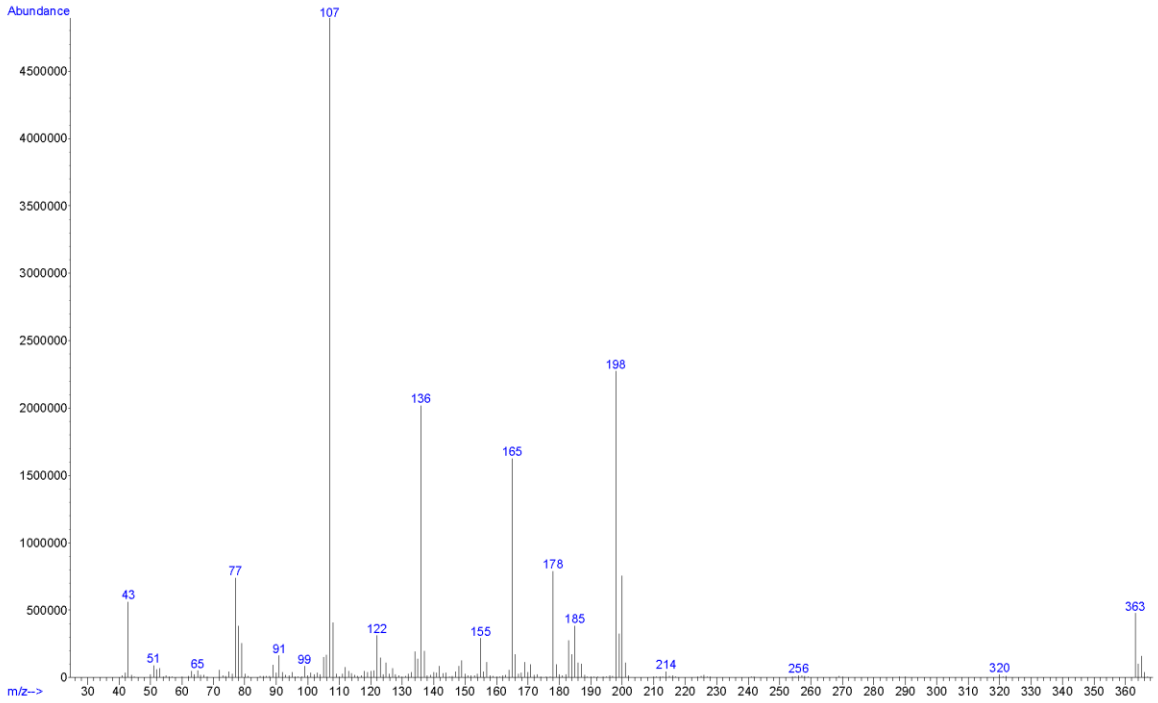


Chromatogram: 25C-NBOH Derivatives (Seized Exhibit - Derivatized)

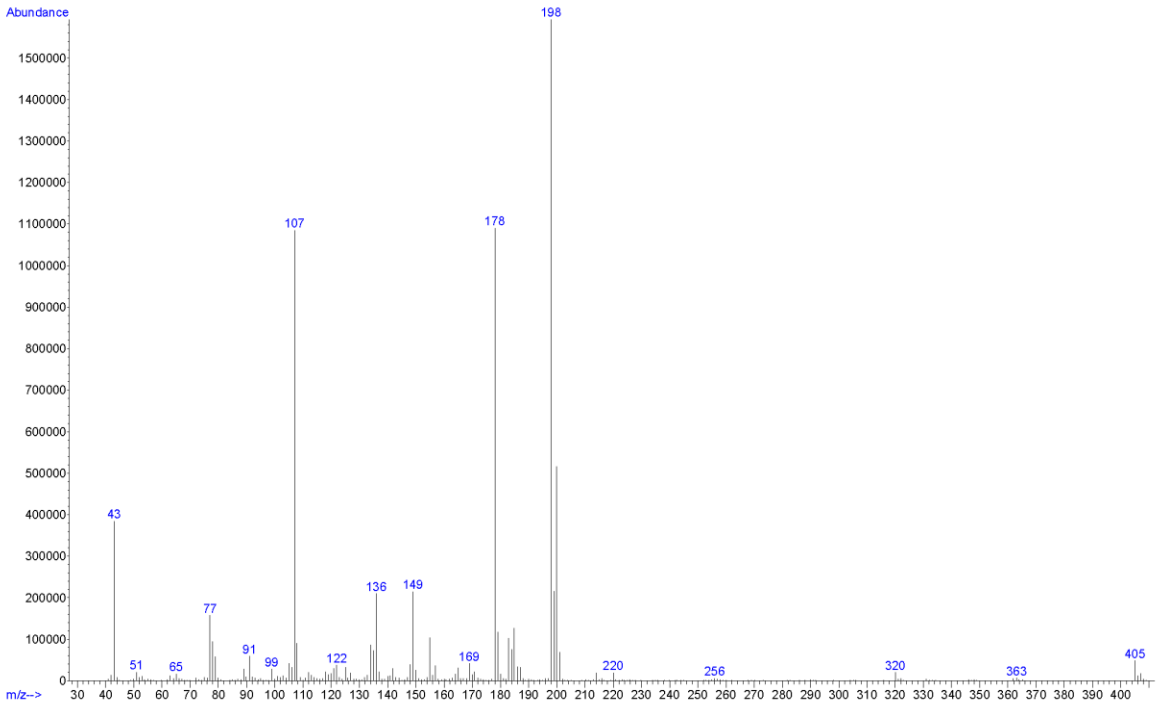


Additional peaks present in chromatogram: internal standard monoacetyl- derivative (4.640 min), internal standard (5.771 min), 25C-NBOH monoacetyl- derivative (8.118 min), 25C-NBOH diacetyl- derivative (8.171 min)

EI (70 eV) Mass Spectrum: 25C-NBOH Monoacetyl- Derivative



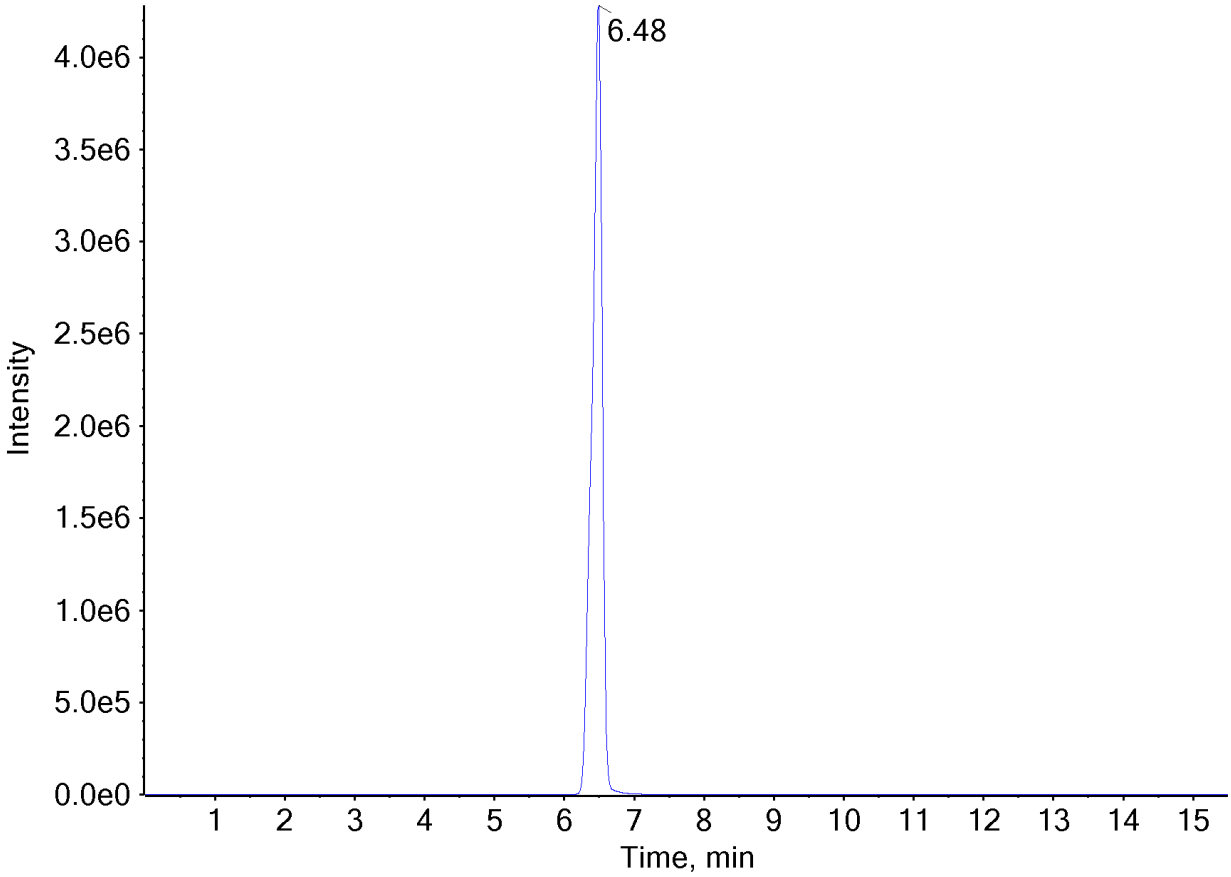
EI (70 eV) Mass Spectrum: 25C-NBOH Diacetyl- Derivative



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 extract in mobile phase (25C-NBOH)
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:	6.48 min
Standard Comparison:	Reference material for 25C-NBOH (Batch: 0464724-22) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 25C-NBOH, based on retention time (6.58 min) and mass spectral data. (https://www.caymanchem.com/product/14815)

Chromatogram: 25C-NBOH



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