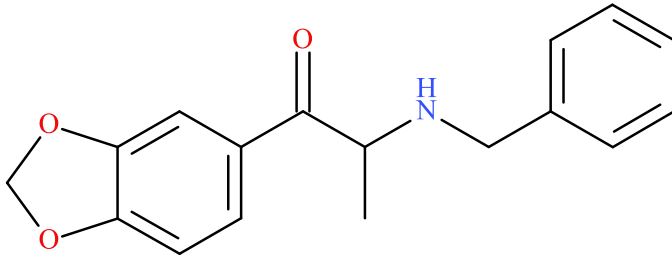


Benzylone (BMDP)

Sample Type: **Seized Material**



Latest Revision: **July 22, 2019**

Date Received: **May 7, 2019**

Date of Report: **June 4, 2019**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(benzylamino)propan-1-one
InChI String:	InChI=1S/C17H17NO3/c1-12(18-10-13-5-3-2-4-6-13)17(19)14-7-8-15-16(9-14)21-11-20-15/h2-9,12,18H,10-11H2,1H3
CFR:	Not Scheduled (06/2019)
CAS#	1823274-68-5
Synonyms:	BMDP, N-benzyl methylene, 3,4-Methylenedioxy-N-benzylcathinone, N-benzyl-3,4-methylenedioxcathinone
Source:	Department of Homeland Security
Appearance:	Pink Solid Material

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

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 ₁₇ NO ₃	283.3	283	284.1281

3. BRIEF DESCRIPTION

Benzyllone (BMDP) 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 methylone, ethylone, butylone, and tertylone, among others. Methylone, butylone, and ethylone (a positional isomer of butylone) are Schedule I substances in the United States; however, benzyllone is not scheduled.

Benzyllone was first reported to the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA) in December of 2010 by a laboratory in the United Kingdom.¹ Additionally, benzyllone has been characterized and reported in the scientific literature.² While this is not the first identification of benzyllone internationally, its increasing prevalence in seized drug casework has prompted interest among forensic science and public health communities.

NMS Labs identified benzyllone in ten seized drug exhibits in May of 2019 from international ports of entry; all exhibits were positive for benzyllone only. Three laboratories in Florida have identified benzyllone in several seized exhibits (more than 10) in recent months and dating back to late 2018. Two laboratories in South Carolina report identifications of benzyllone in 2019, totaling more than ten seized exhibits as well. One identification of benzyllone was reported from North Dakota in April 2019. In addition to its national spread, benzyllone was recently identified in two exhibits in Australia after a long gap in detection since its first identification in the country in 2013. Several of these laboratories also reported the combination of benzyllone with other emergent cathinones, including [N-butyl pentylone](#) and [eutylone](#), and methamphetamine. The seized exhibits were most commonly described as powders and tablets.

4. ADDITIONAL RESOURCES

1. EMCDDA–Europol 2010 Annual Report on the implementation of Council Decision 2005/387/JHA. http://www.emcdda.europa.eu/publications/implementation-reports/2010_en

2. Fornal, E; Stachniuk, A; Wojtyla, A. LC-Q/TOF mass spectrometry data driven identification and spectroscopic characterisation of a new 3,4-methylenedioxy-N-benzyl cathinone (BMDP). *J Pharm Biomed Anal.* **2013**; 72:139-44.

<https://www.ncbi.nlm.nih.gov/pubmed/23146238>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/BMDP-ID-1875-17_report.pdf

<https://www.caymanchem.com/product/9001330>

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: Zebtron™ 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

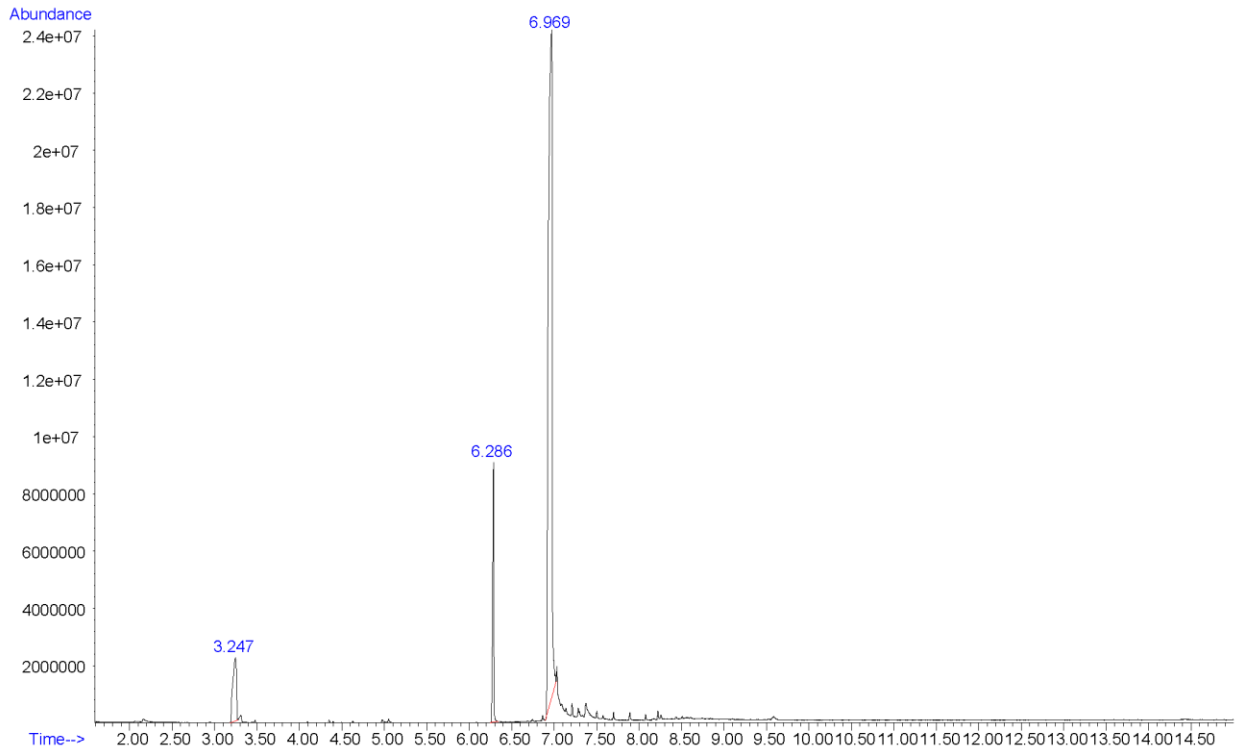
Retention Time: 6.969 min

Standard Comparison:

Reference material for benzylone (Batch: 0448208-15) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as benzylone, based on retention time (6.927 min) and mass spectral data.

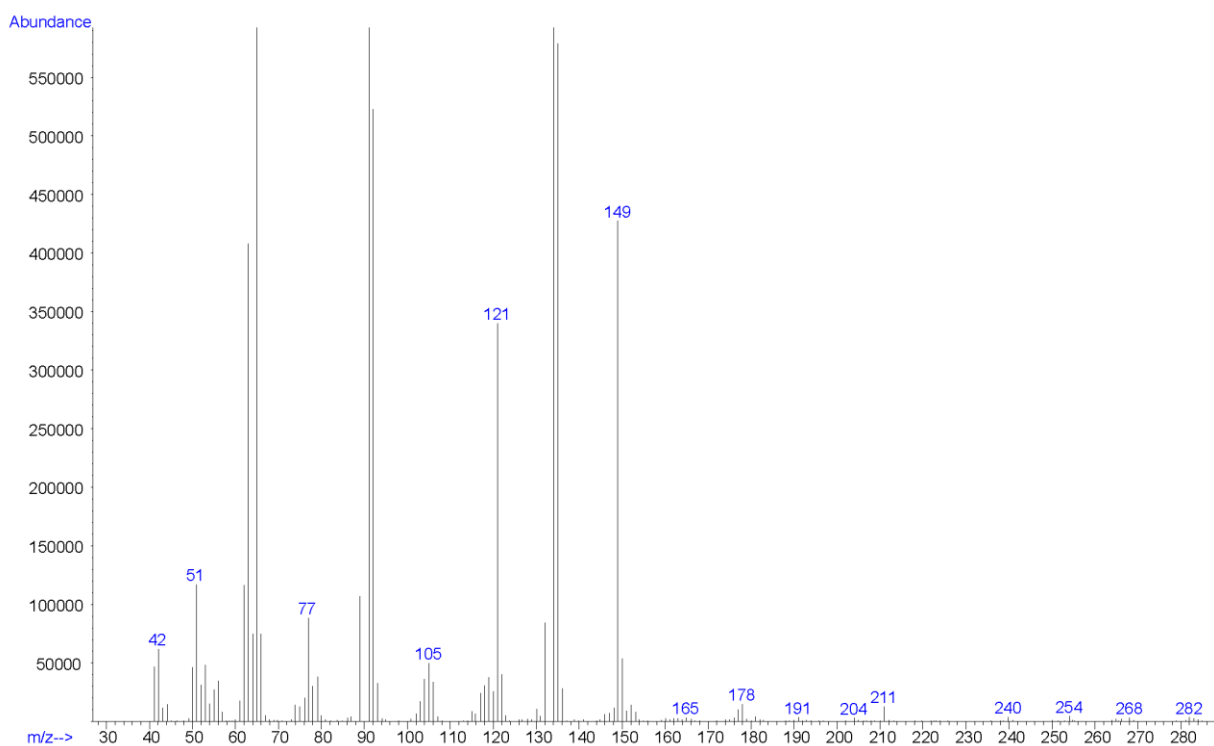
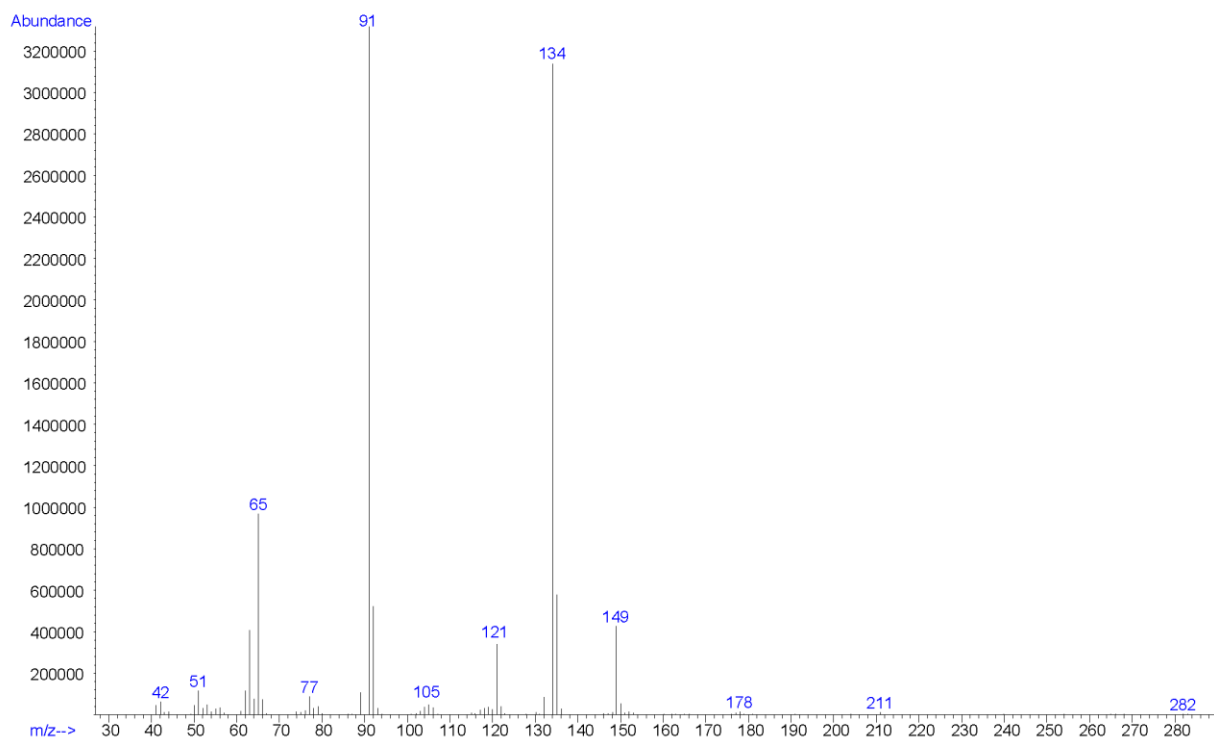
<https://www.caymanchem.com/product/9001330>

Chromatogram: Benzylone



Additional peaks present in chromatogram: internal standards (3.247 min and 6.286 min)

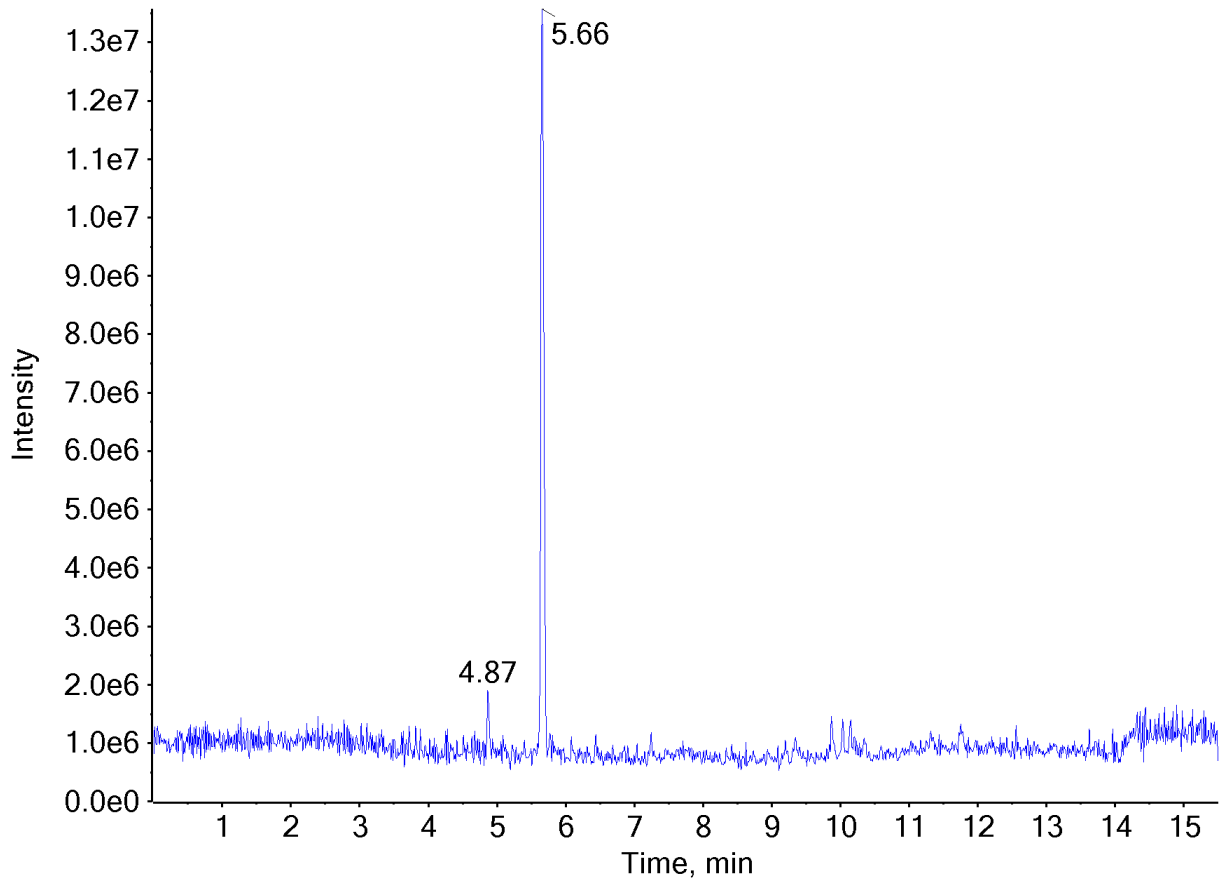
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Benzylone



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

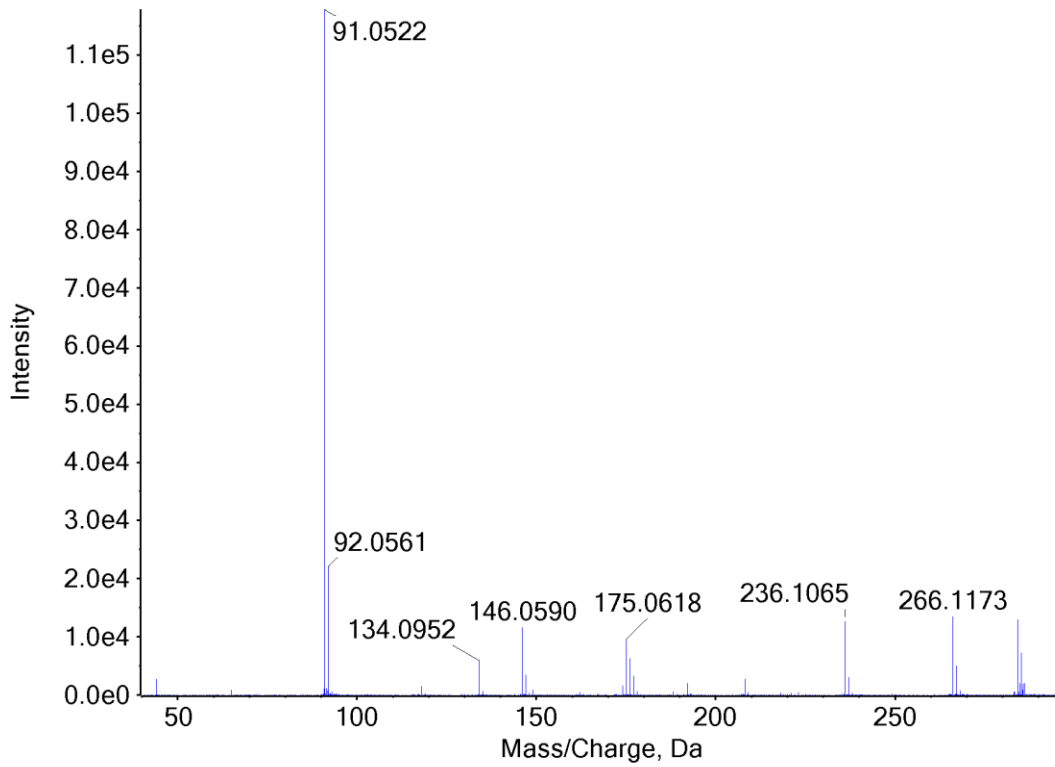
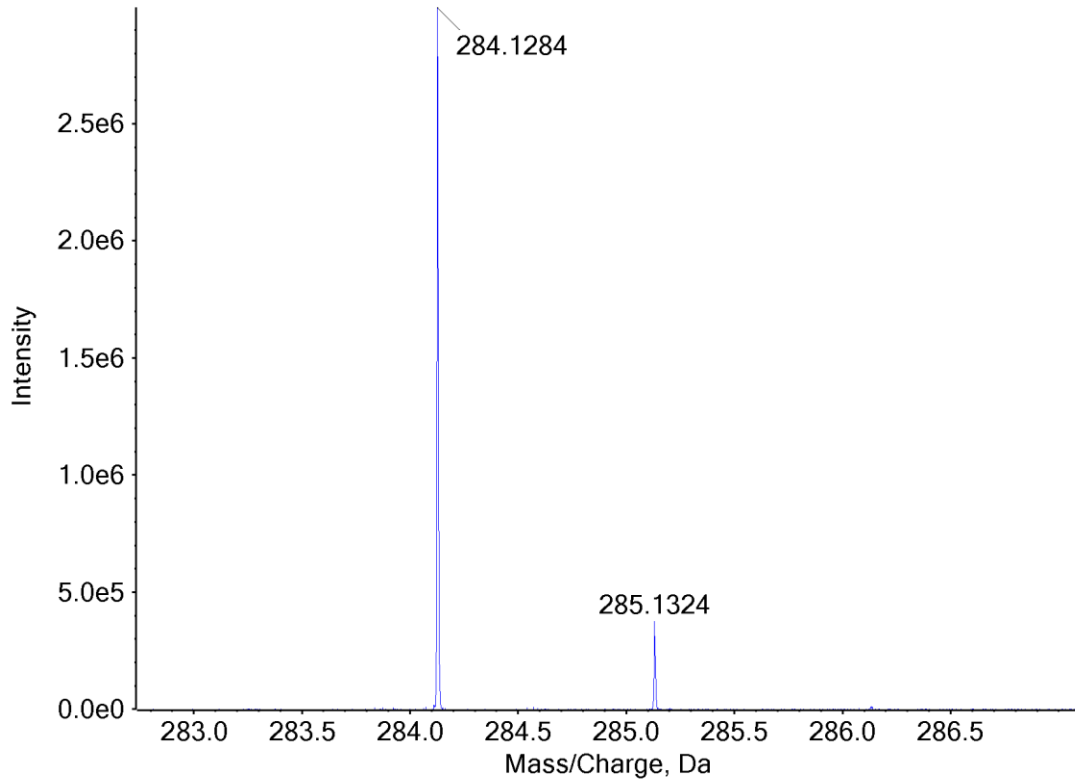
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	5.66 min
Standard Comparison:	Reference material for benzylone (Batch: 0448208-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as benzylone, based on retention time (5.71 min) and mass spectral data. (https://www.caymanchem.com/product/9001330)

Chromatogram: Benzylone



Additional peaks present in chromatogram: internal standard (4.87 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Benzylone



6. ACKNOWLEDGEMENT

The authors of this monograph would like to acknowledge the SYNTH-OPIOIDS listserv, administered by Agnes Winokur, for feedback and contributions, specifically Carlene Rittenbach of the North Dakota Office of Attorney General; Karen Blakey of Queensland Health Forensic and Scientific Services (QHFSS) in Australia; Renee Hilton of the City of Charleston Police Department, South Carolina; the Miami-Dade Police Department in Florida; Reta Newman of the Pinellas County Forensic Lab in Florida; Jessi Ziepfel of the Beaufort County Sheriff's Office in South Carolina; and Julie Bacigalupi of the Broward County Sherriff's Office in Florida.

7. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
07/22/2019	Important Note (Page 1) Revised: "All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material."