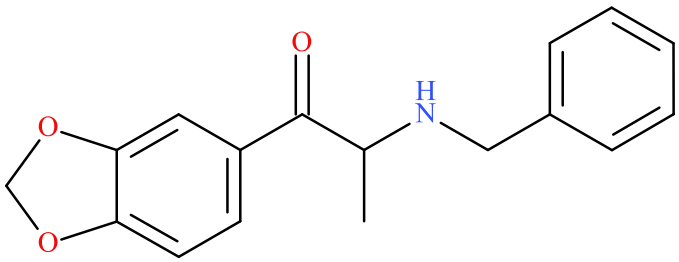
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

Benzylone (BMDP)



Sample Type: **Seized Material**

Latest Revision: **June 4, 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 methylone, 3,4-Methylenedioxy-N-benzylcathinone, N-benzyl-3,4-methylenedioxycathinone
Source:	Department of Homeland Security
Appearance:	Pink 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.*

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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

Benzylone (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, benzylone is not scheduled.

Benzylone 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, benzylone has been characterized and reported in the scientific literaute.[2] While this is not the first identification of benzylone internationally, its increasing prevalence in seized drug casework has prompted interest among forensic science and public health communities.

NMS Labs identified benzylone in ten seized drug exhibits in May of 2019 from international ports of entry; all exhibits were positive for benzylone only. Three laboratories in Florida have identified benzylone in several seized exhibits (more than 10) in recent months and dating back to late 2018. Two laboratories in South Carolina report identifications of benzylone in 2019, totaling more than ten seized exhibits as well. One identification of benzylone was reported from North Dakota in April 2019. In addition to its national spread, benzylone 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 benzylone 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

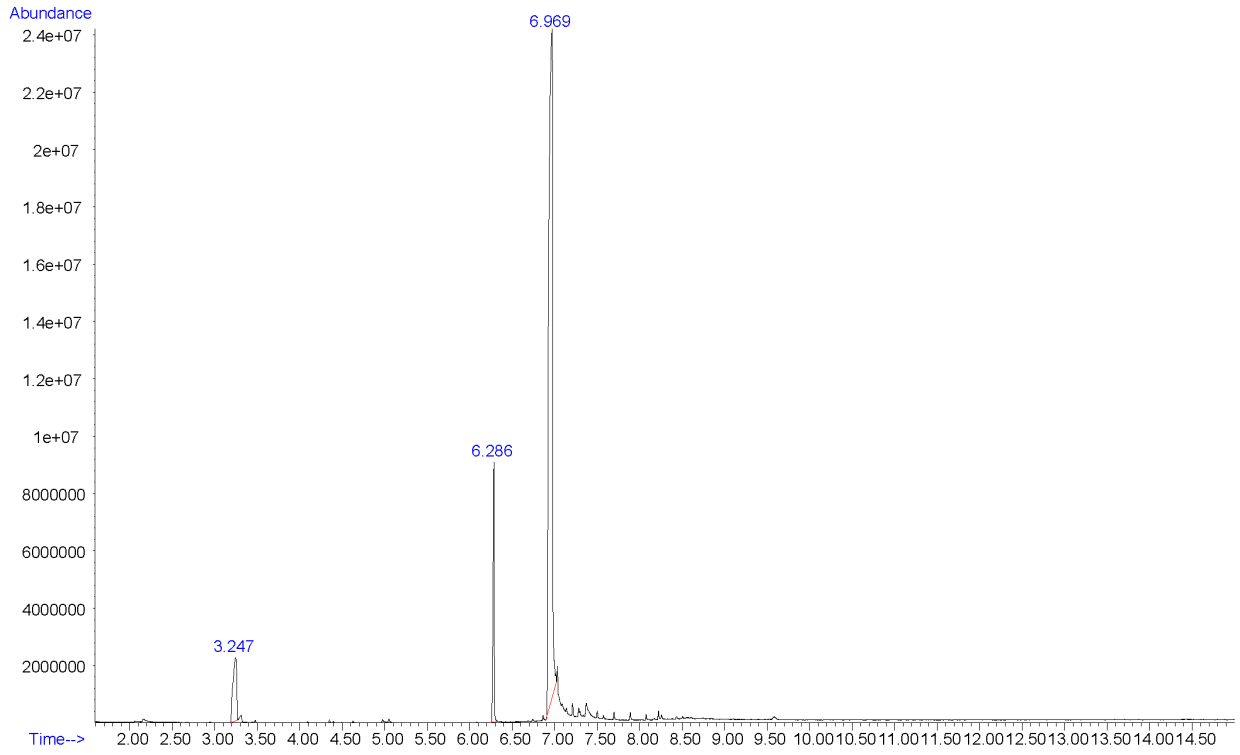
5. QUALITATIVE DATA

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:	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:	6.969 min

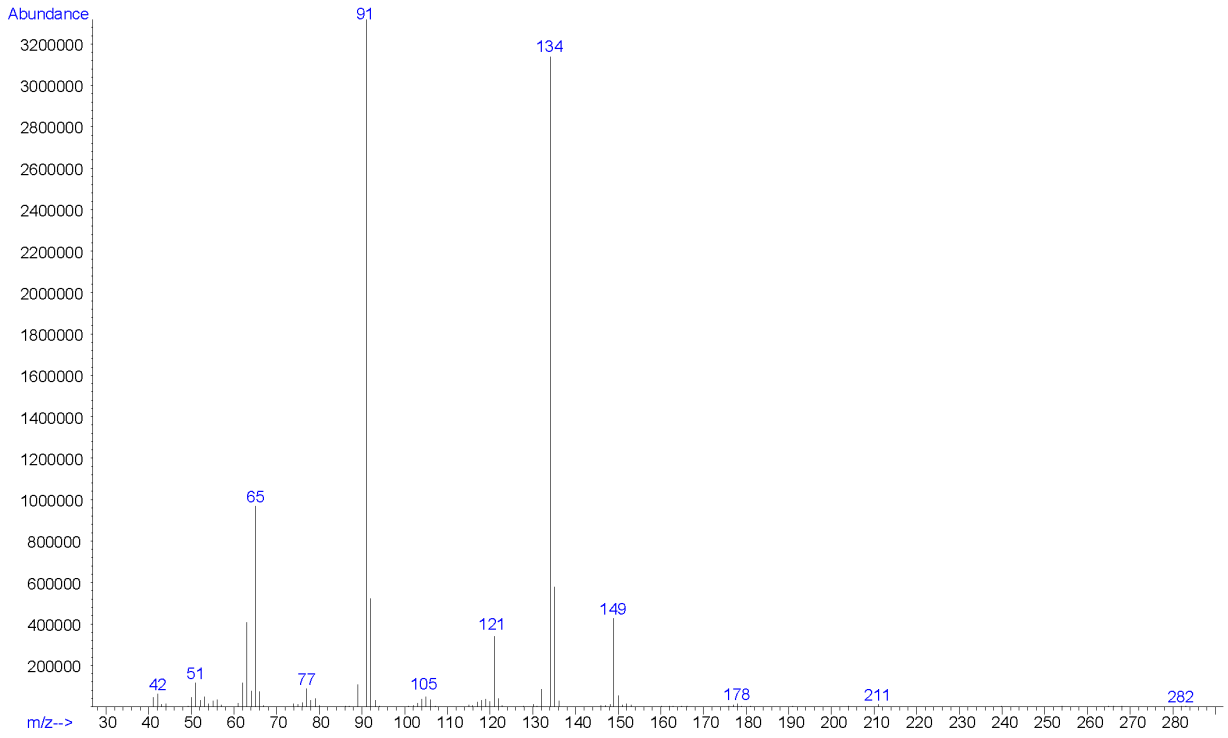
Standard Comparison: Reference material for benzylone (Batch: 0448208-15) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as benzylone, based on retention time (6.927 min) and mass spectral data. (https://www.caymanchem.com/product/9001330)

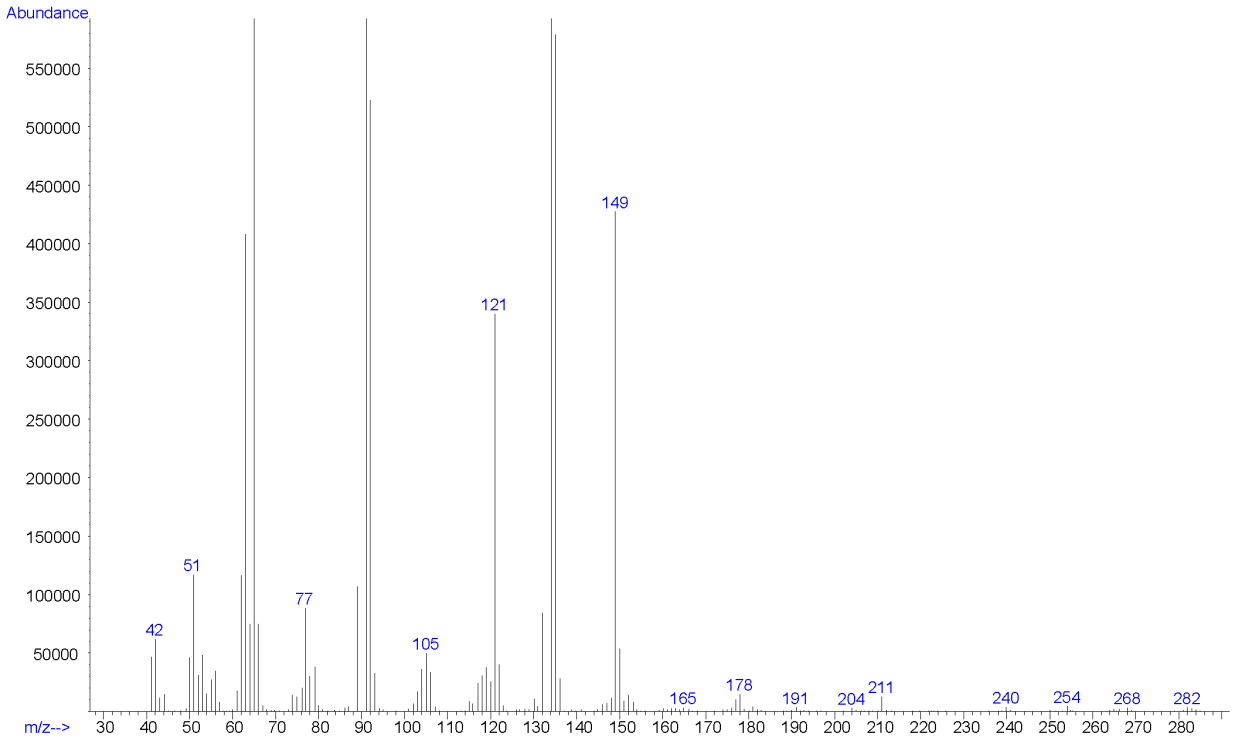
Chromatogram: Benzylone



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

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

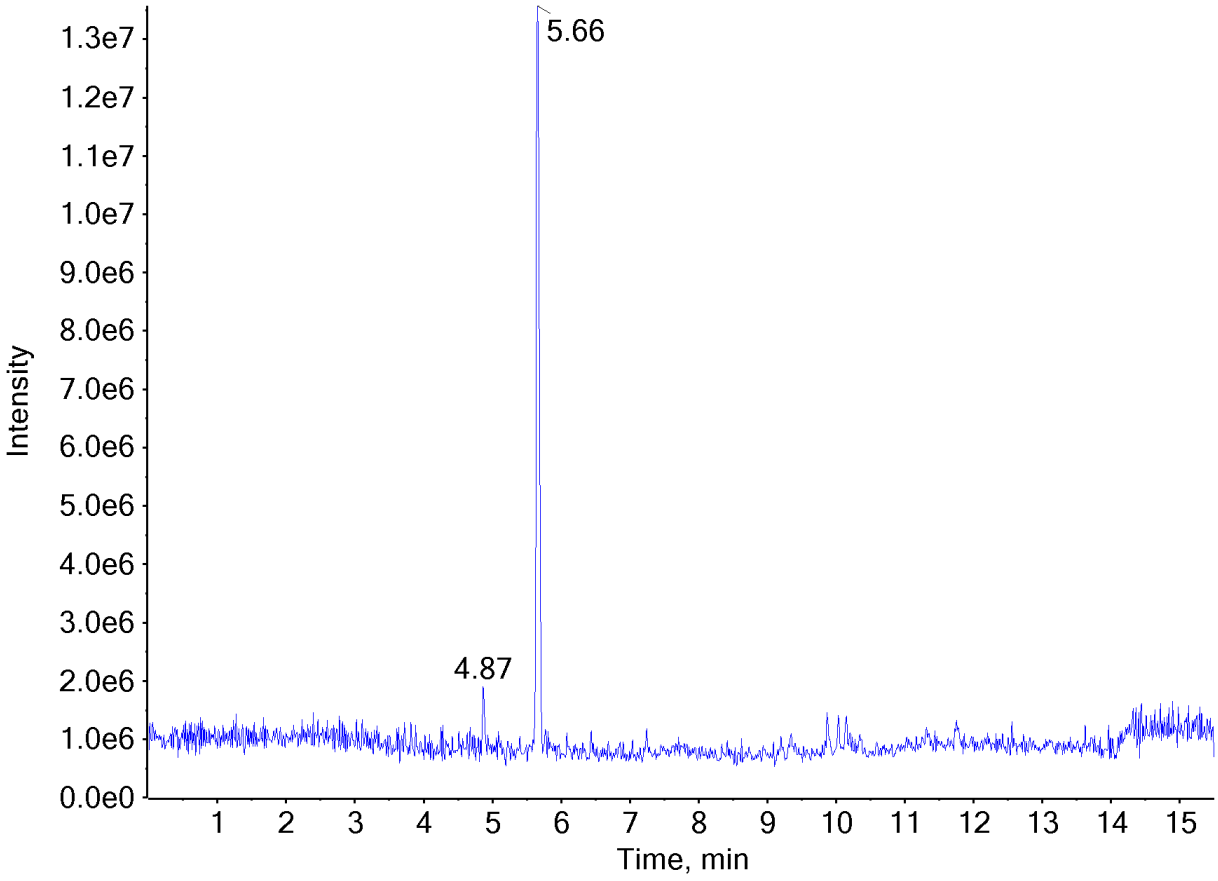




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

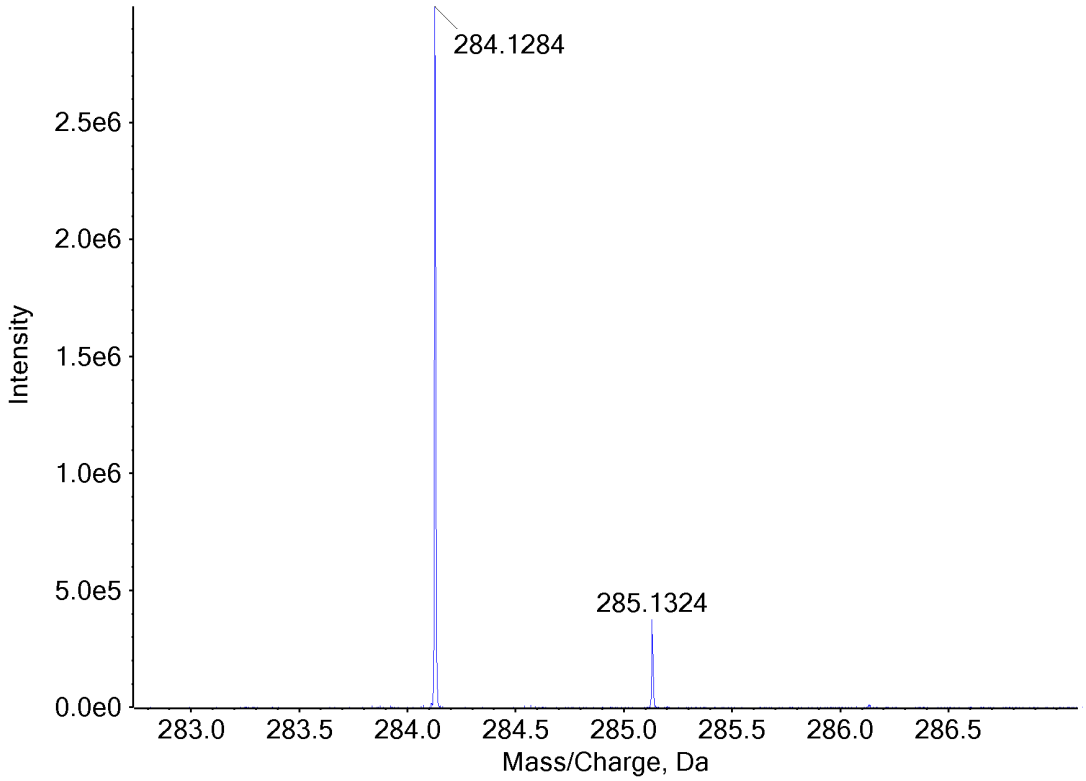
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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: Collison 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)

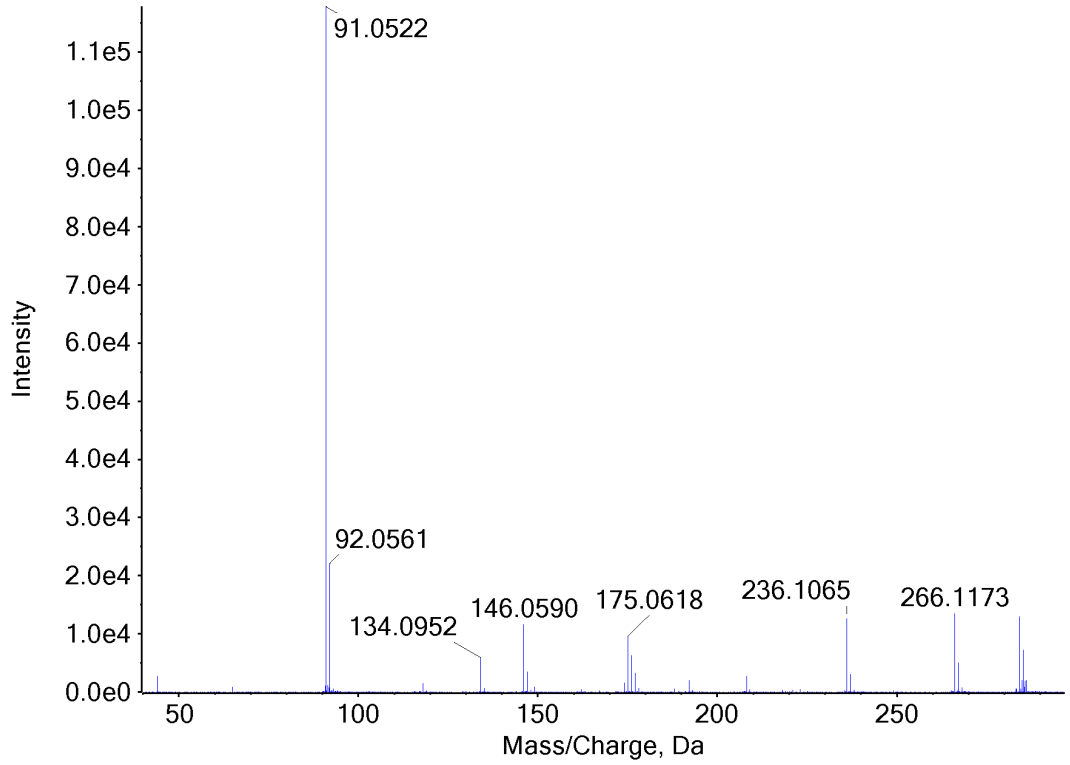
Chromatogram: Benzylone



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

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





6. ACKNOWLEDGEMENT

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