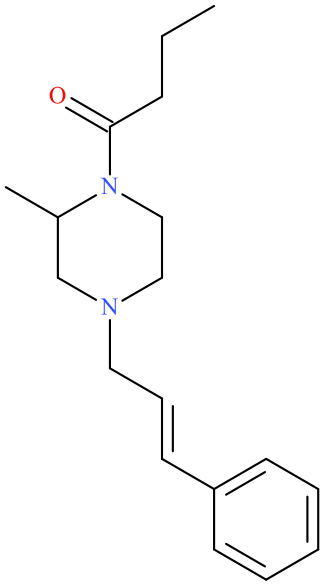
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

2-Methyl AP-237



Sample Type: **Seized Material**

Latest Revision: **July 22, 2019**

Date Received: **May 7, 2019**

Date of Report: **June 21, 2019**

1. GENERAL INFORMATION

IUPAC Name:	1-[4-[(E)-cinnamyl]-2-methyl-piperazin-1-yl]butan-1-one
InChI String:	InChI=1S/C18H26N2O/c1-3-8-18(21)20-14-13-19(15-16(20)2)12-7-11-17-9-5-4-6-10-17/h4-7,9-11,16H,3,8,12-15H2,1-2H3/b11-7+
CFR:	Not Scheduled (06/2019)
CAS#	98608-59-4
Synonyms:	2-methyl Bucinnazine
Source:	Department of Homeland Security
Appearance:	White 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	$C_{18}H_{26}N_2O$	286.4	286	287.2118

3. BRIEF DESCRIPTION

2-Methyl AP-237 is classified as a synthetic opioid. 2-Methyl AP-237 is structurally distinct from fentanyl, its analogues, and other synthetic opioids previously reported. 2-Methyl AP-237 is an analogue of bucinnazine (AP-237), an opioid used therapeutically; although bucinnazine is not prescribed within the United States. Based on its recent emergence and potential for abuse within the United States and worldwide, 2-methyl AP-237 has been categorized as a Novel Psychoactive Substance (NPS). 2-Methyl AP-237 and bucinnazine are not scheduled substances in the United States. 2-Methyl AP-237 was found to be active, having both central and peripheral analgesic activity.[1]

4. ADDITIONAL RESOURCES

1. Methyl-piperazino derivatives with analgesic activity, a process for their preparation, and therapeutic compounds which contain them. Furlan, D. EURORESEARCH S.R.L. EP0142756A2. 1985. https://patents.google.com/patent/EP0142756A2/en

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/2-Methyl-AP-237-ID-2053-19_report.pdf

https://www.caymanchem.com/product/26485

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

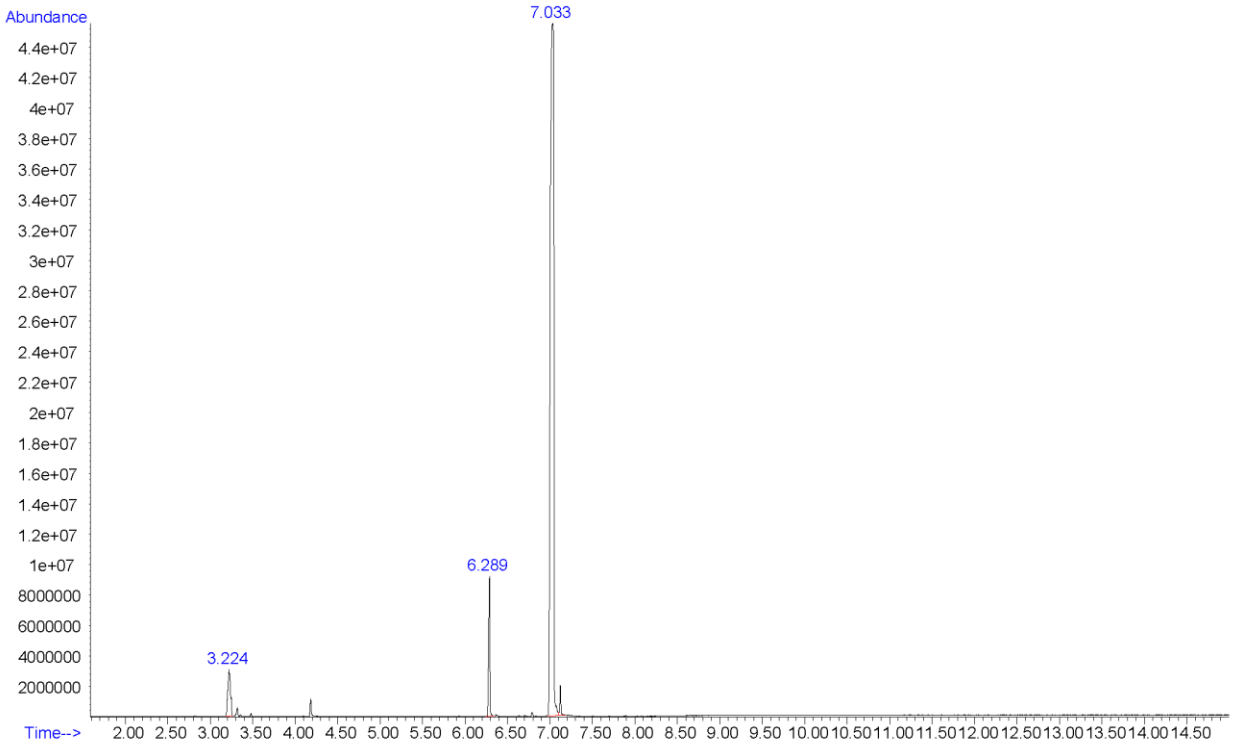
Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

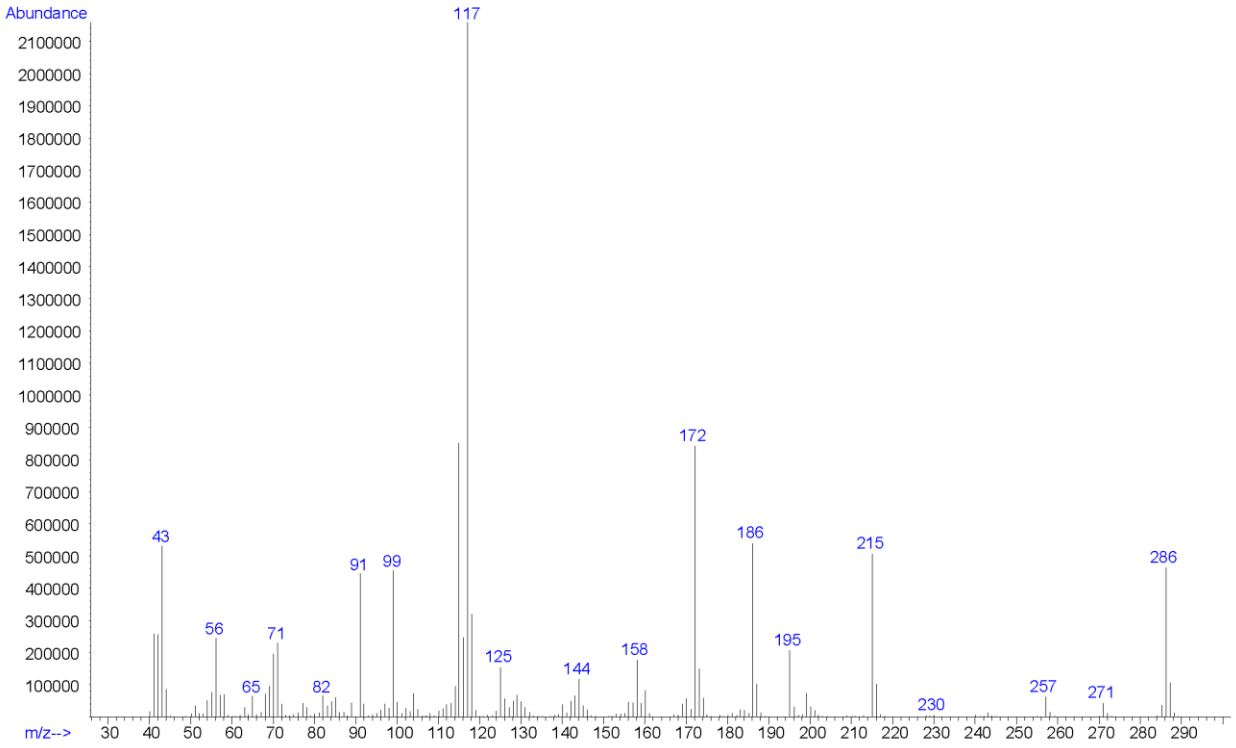
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	7.033 min
Standard Comparison:	Reference material for 2-methyl AP-237 (Batch: 0545937-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 2-methyl AP-237, based on retention time (6.995 min) and mass spectral data. (https://www.caymanchem.com/product/26485)

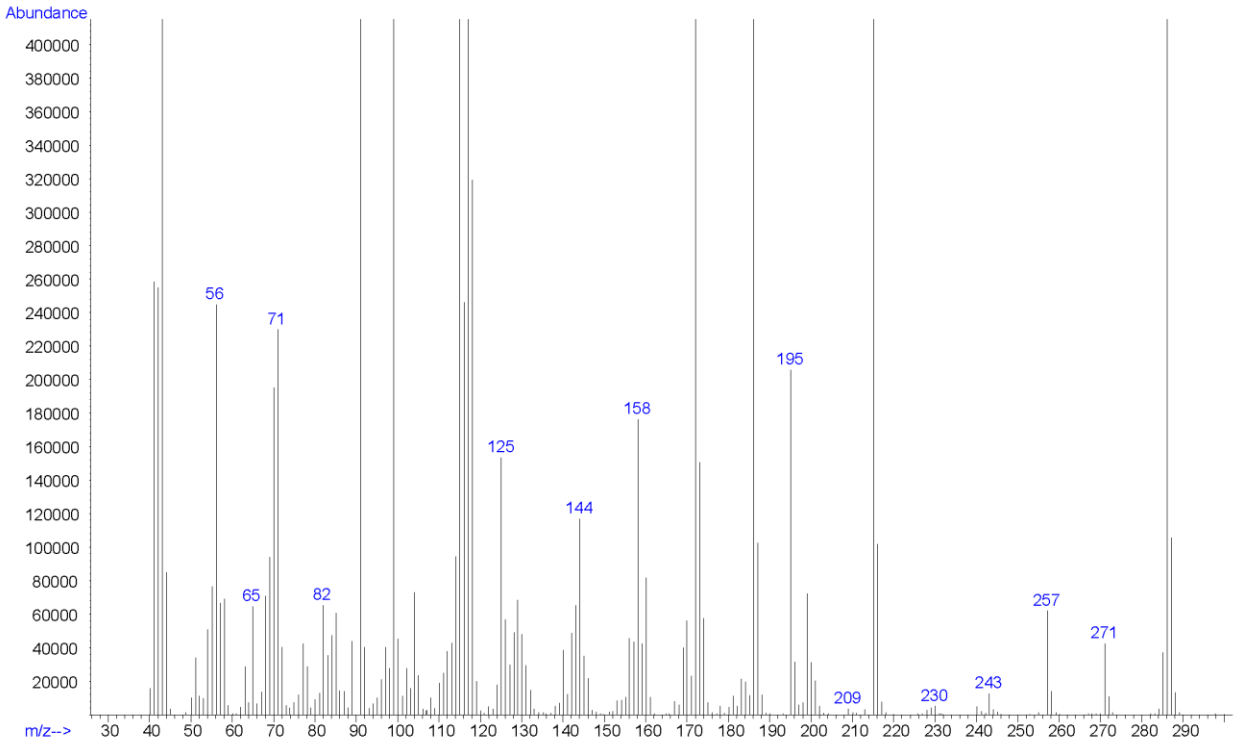
Chromatogram: 2-Methyl AP-237



Additional peaks present in chromatogram: internal standards (3.224 min and 6.289 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 2-Methyl AP-237

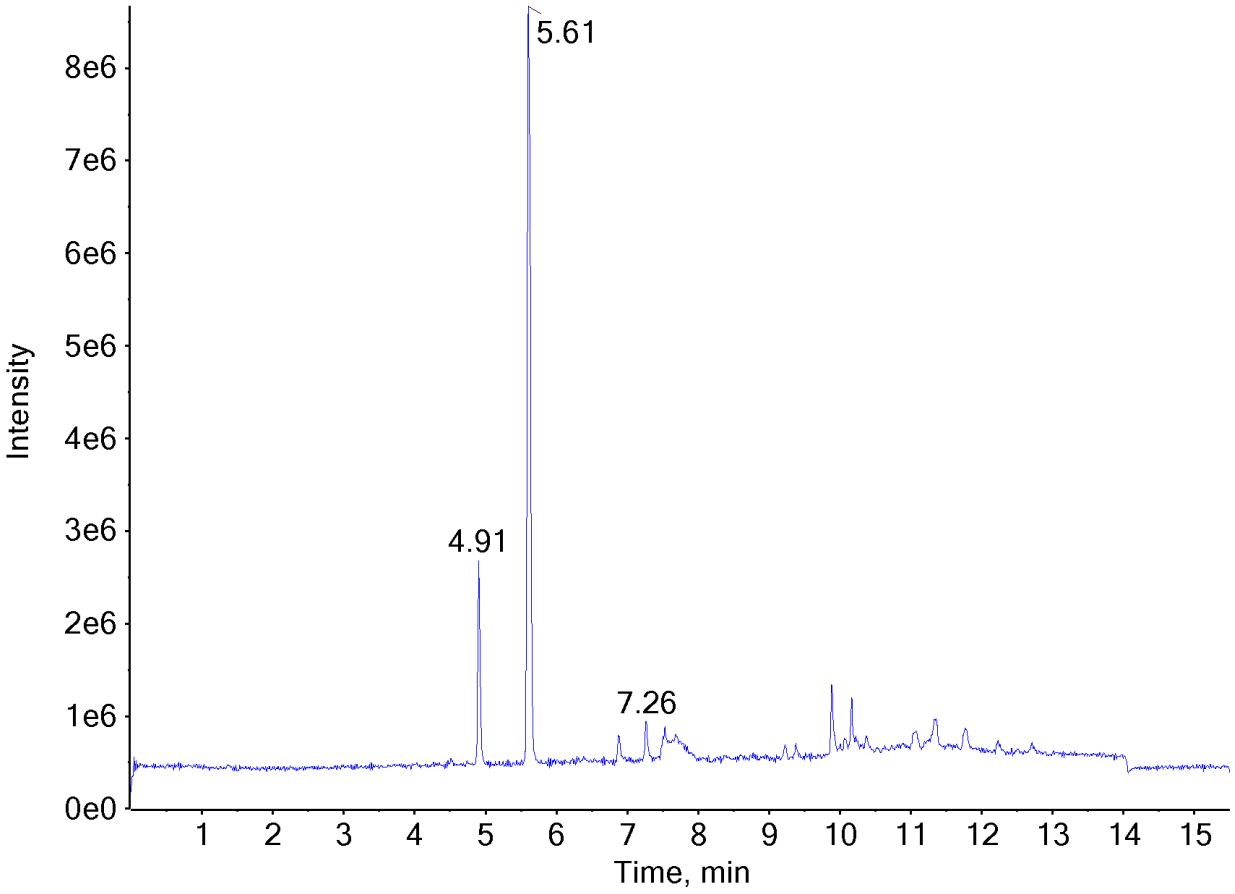




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

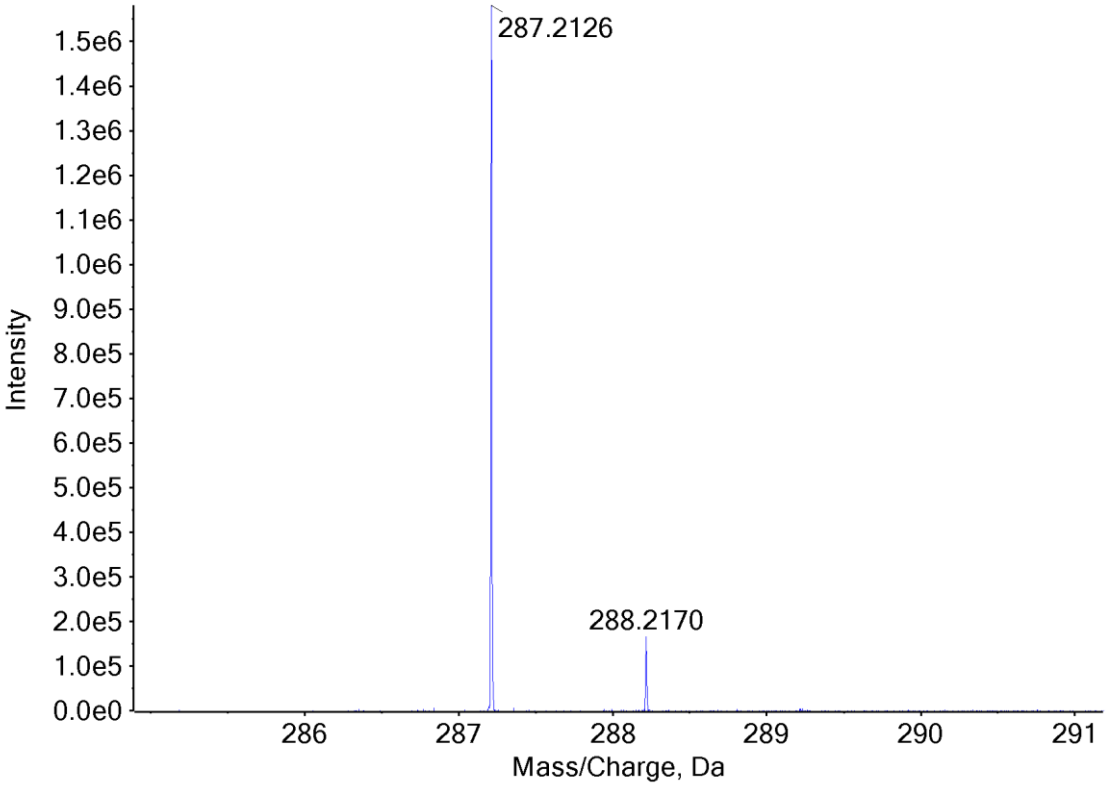
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	5.61 min
Standard Comparison:	Reference material for 2-methyl AP-237 (Batch: 0545937-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 2-methyl AP-237, based on retention time (5.61 min) and mass spectral data. (https://www.caymanchem.com/product/26485)

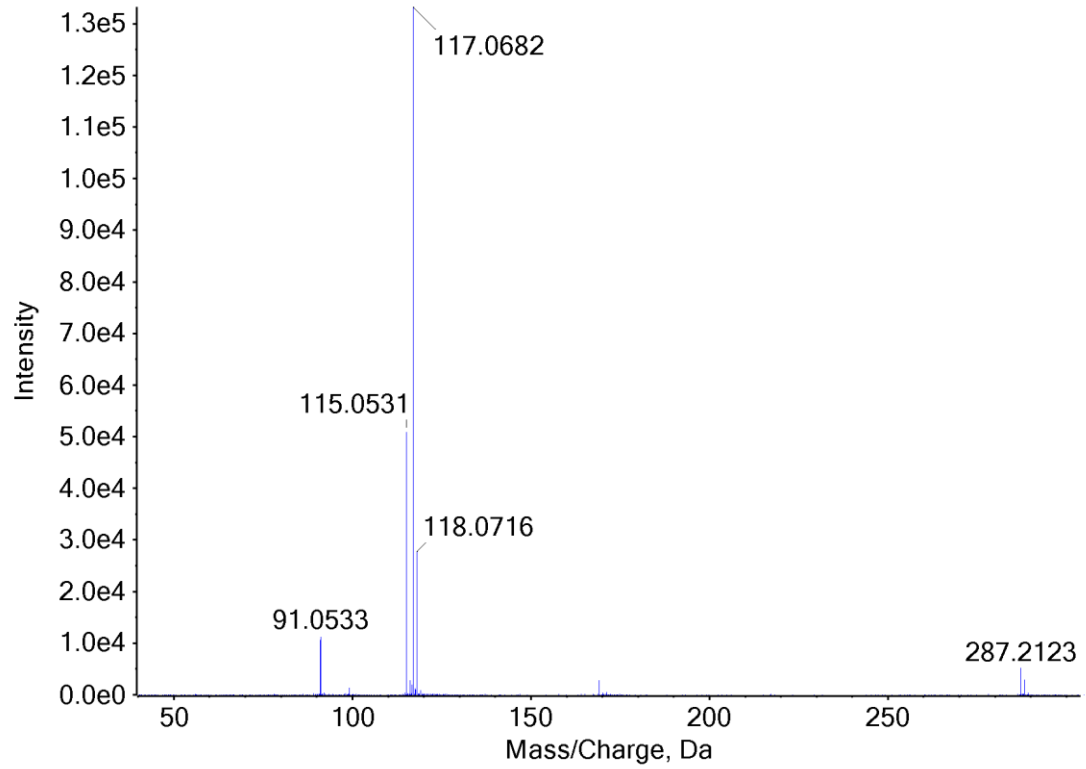
Chromatogram: 2-Methyl AP-237



Additional peaks present in chromatogram: internal standards (4.91 min and 7.26 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 2-Methyl AP-237





6. REVISION HISTORY

Date	Revision
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.”