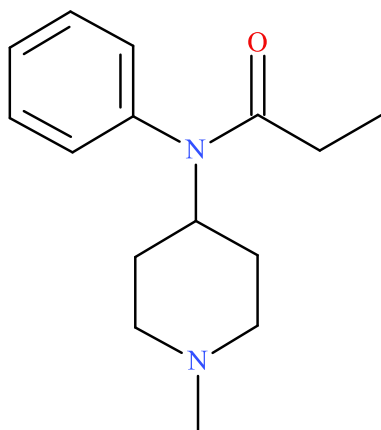


N-methyl Norfentanyl

 Latest Revision: **April 13, 2018**

 Date Received: **February 12, 2018**

 Date of Report: **April 10, 2018**


1. GENERAL INFORMATION

IUPAC Name:	N-(1-methyl-4-piperidyl)-N-phenyl-propanamide
InChI String:	InChI=1S/C15H22N2O/c1-3-15(18)17(13-7-5-4-6-8-13)14-9-11-16(2)12-10-14/h4-8,14H,3,9-12H2,1-2H3
CFR:	Not Scheduled (04/2018)
CAS#	24775-71-1
Synonyms:	Not applicable
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 ₁₅ H ₂₂ N ₂ O	246.35	246	247.1805

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.

3. BRIEF DESCRIPTION

N-methyl norfentanyl is classified as a suspected fentanyl precursor. Fentanyl precursors are modified based on the structure of fentanyl with the absence of notable functional groups or structural features. Fentanyl precursors are often used in the synthesis of fentanyl and its analogues. *N*-methyl norfentanyl has been determined in a mouse model to be inactive¹.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/24446>

1. Schneider, E. & Brune, K. [Opioid activity and distribution of fentanyl metabolites](#). *Naunyn-Schmiedeberg's Arch. Pharmacol.* (1986) 334: 267.

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

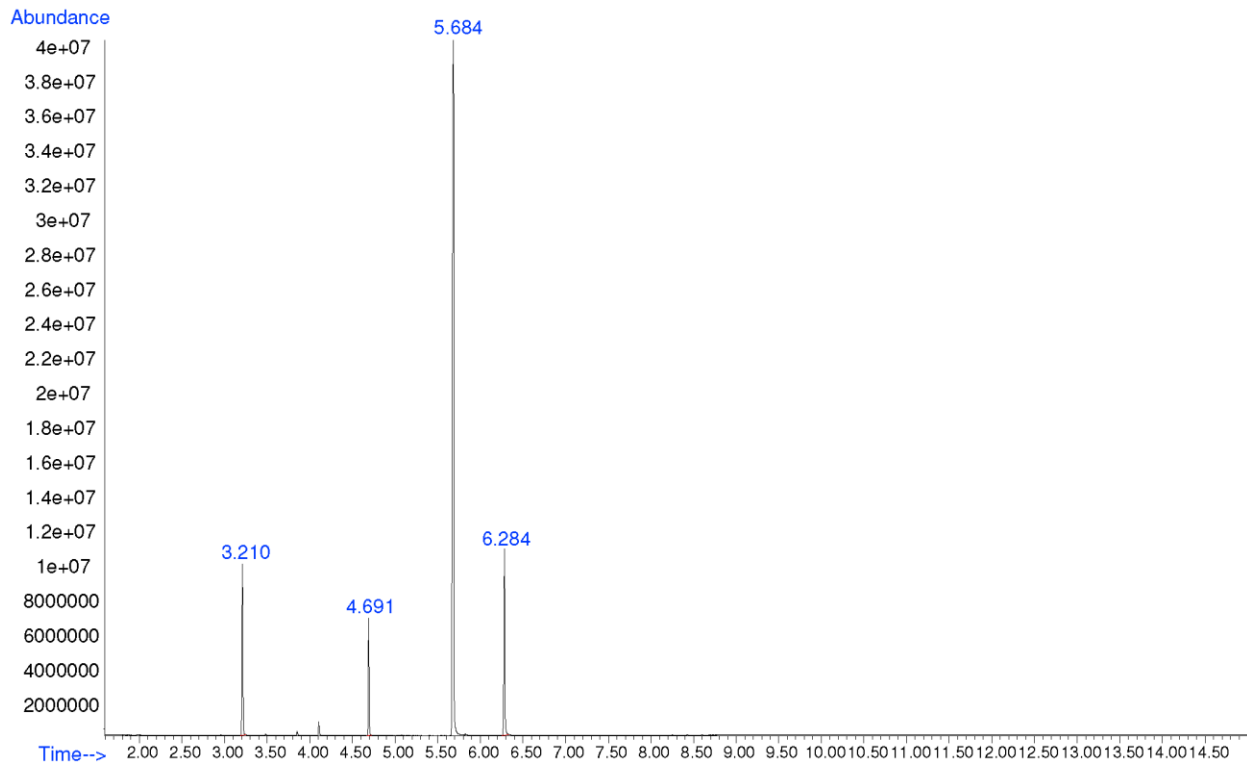
Injection Parameters:
Injection Type: Splitless
Injection Volume: 1 μL

MS Parameters:
Mass Scan Range: 40-550 m/z
Threshold: 250

Retention Time: 5.684 min

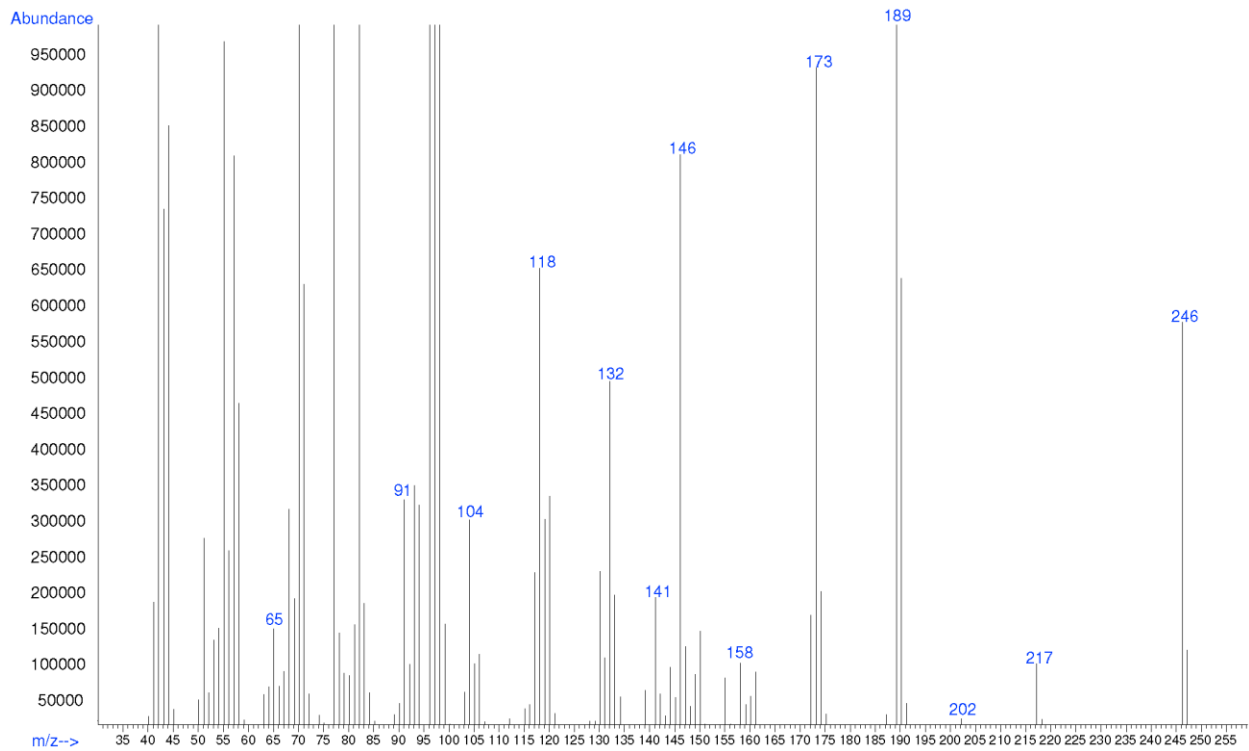
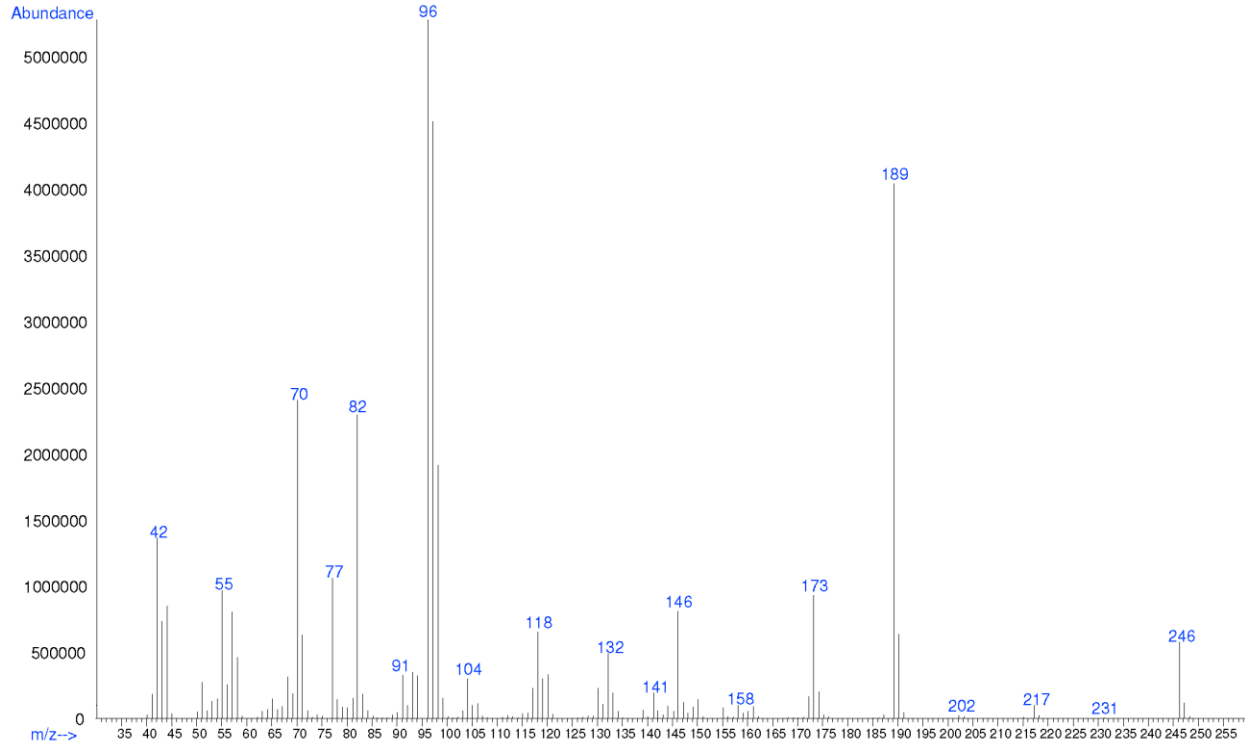
Standard Comparison: Reference material for *N*-methyl norfentanyl (Batch: 0524407-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-methyl norfentanyl, based on retention time (5.682 min) and mass spectral data.
(<https://www.caymanchem.com/product/24446>)

Chromatogram: *N*-methyl Norfentanyl



Additional peaks present in chromatogram: internal standard 1 (3.210 min), not a controlled substance (4.691 min), internal standard 2 (6.284 min)

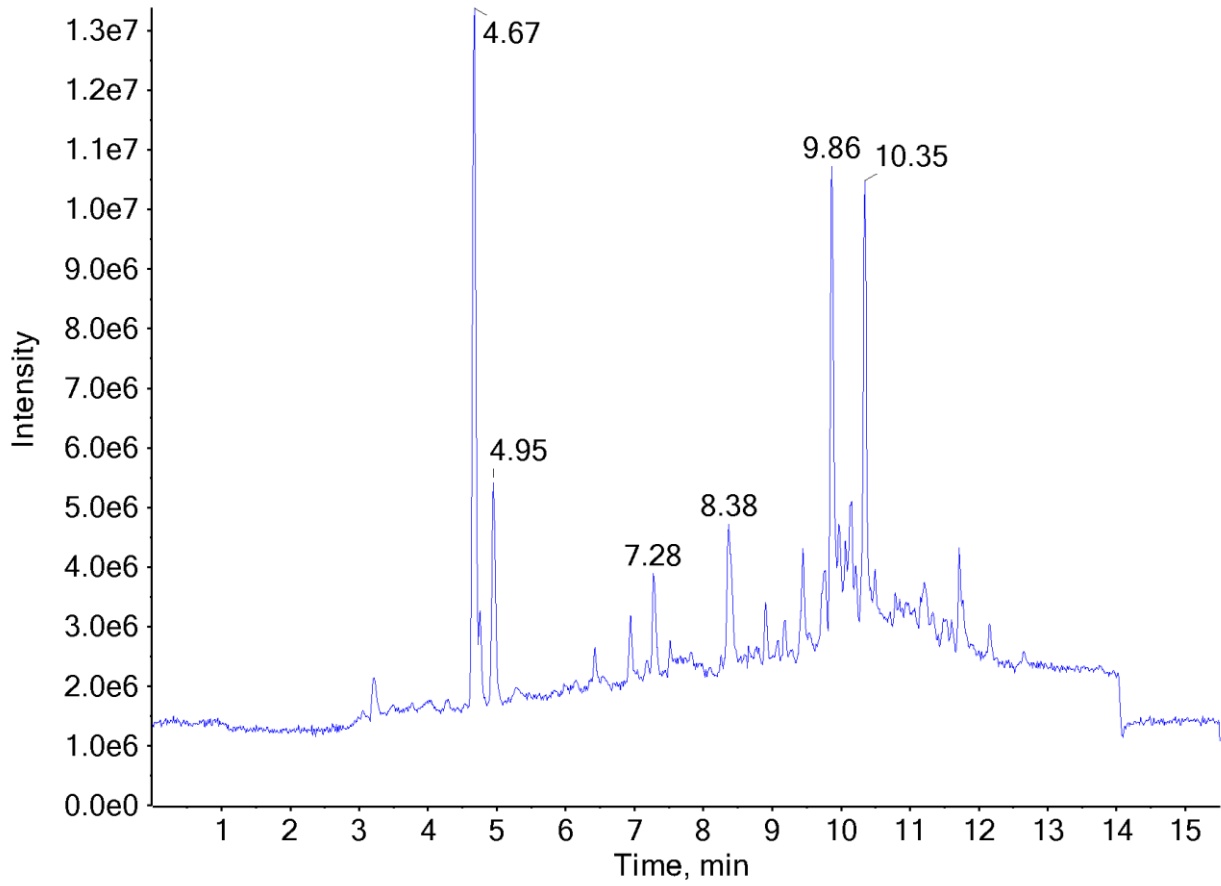
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-methyl Norfentanyl



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

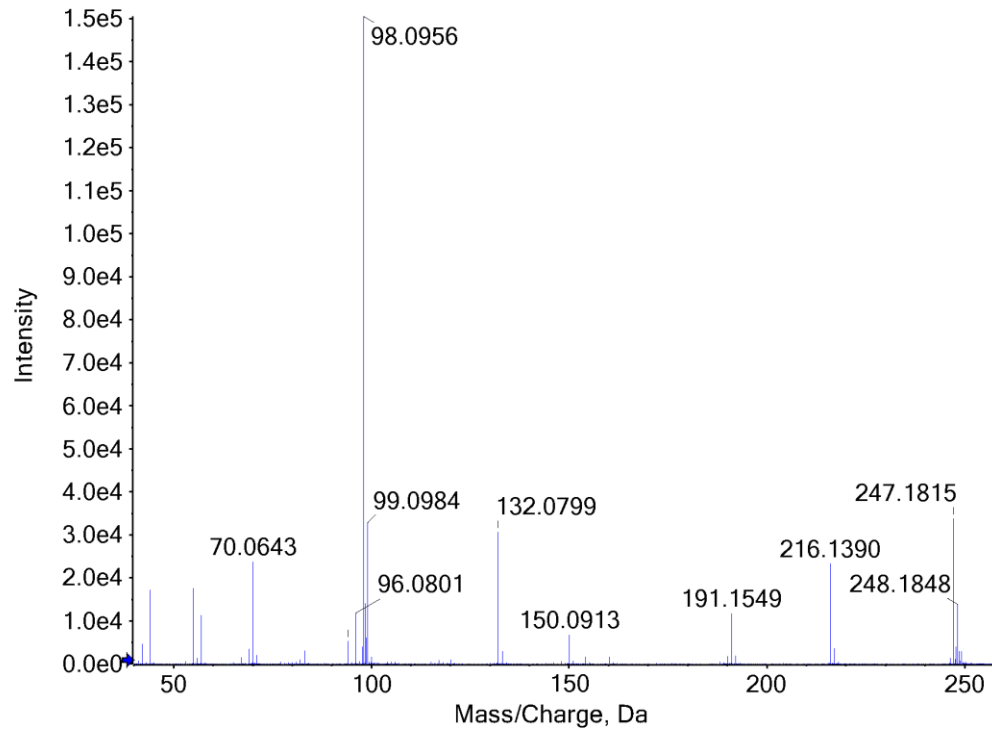
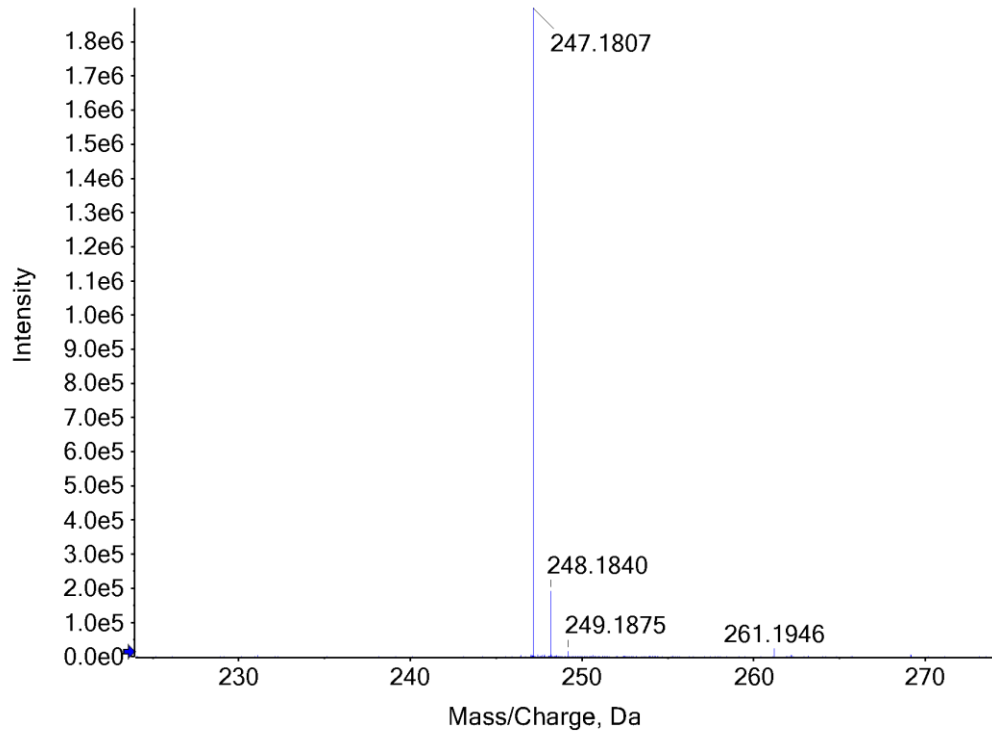
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	4.67 min
Standard Comparison:	Reference material for <i>N</i> -methyl norfentanyl (Batch: 0524407-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as <i>N</i> -methyl norfentanyl, based on retention time (4.660 min) and mass spectral data. (https://www.caymanchem.com/product/24446)

Chromatogram: N-methyl Norfentanyl



Additional peaks present in chromatogram: internal standard 1 (4.95 min), internal standard 2 (7.28 min), not a controlled substance (8.38 min), not a controlled substance (9.86 min), not a controlled substance (10.35 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: N-methyl Norfentanyl



6. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
04/13/2018	Added Additional Resource: "1. Schneider, E. & Brune, K. Opioid activity and distribution of fentanyl metabolites. Naunyn-Schmiedeberg's Arch. Pharmacol. (1986) 334: 267."