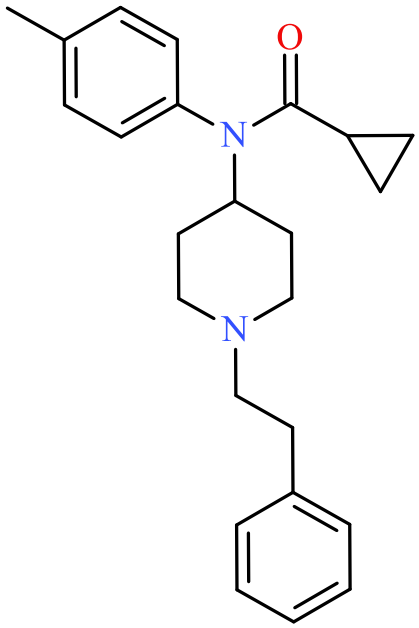
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

para-Methylcyclopropylfentanyl



Sample Type: **Seized Material**

Latest Revision: **November 26, 2019**

Date Received: **October 3, 2019**

Date of Report: **November 26, 2019**

1. GENERAL INFORMATION

IUPAC Name:	N-[1-(2-phenylethyl)-4-piperidyl]-N-(p-tolyl)cyclopropanecarboxamide
InChI String:	InChI=1S/C24H30N2O/c1-19-7-11-22(12-8-19)26(24(27)21-9-10-21)23-14-17-25(18-15-23)16-13-20-5-3-2-4-6-20/h2-8,11-12,21,23H,9-10,13-18H2,1H3
CFR:	21 CFR 1308: Temporary Placement of Fentanyl-Related Substances in Schedule 1 (02/06/2018)
CAS#	Not Available
Synonyms:	4-Methylcyclopropylfentanyl, *p*-Methyl cyclopropyl fentanyl
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-MS) in comparison to analysis of acquired reference material.*

***Prepared By:** Alex J. Krotulski, PhD; 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	$C_{24}H_{30}N_2O$	362.5	362	363.2431

3. BRIEF DESCRIPTION

para-Methylcyclopropylfentanyl is classified as a fentanyl analogue and novel opioid. Fentanyl analogues are modified based on the structure of fentanyl. Fentanyl analogues have been reported to cause psychoactive effects, similar to fentanyl and other opioids. Fentanyl analogues have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include fentanyl, cyclopropylfentanyl, and other fentanyl analogues. *para*-Methylcyclopropylfentanyl is not explicitly scheduled by name, but recent legislation has temporarily placed all fentanyl-related substances in Schedule I.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/23045

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)

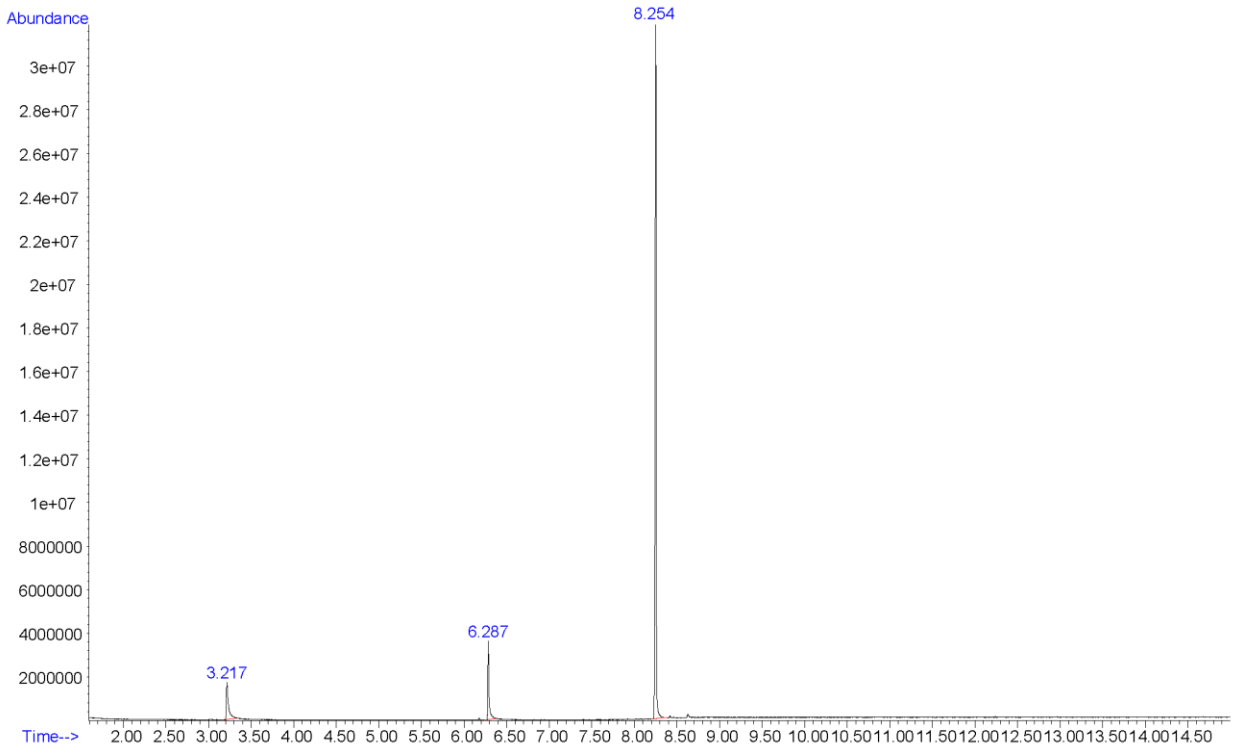
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

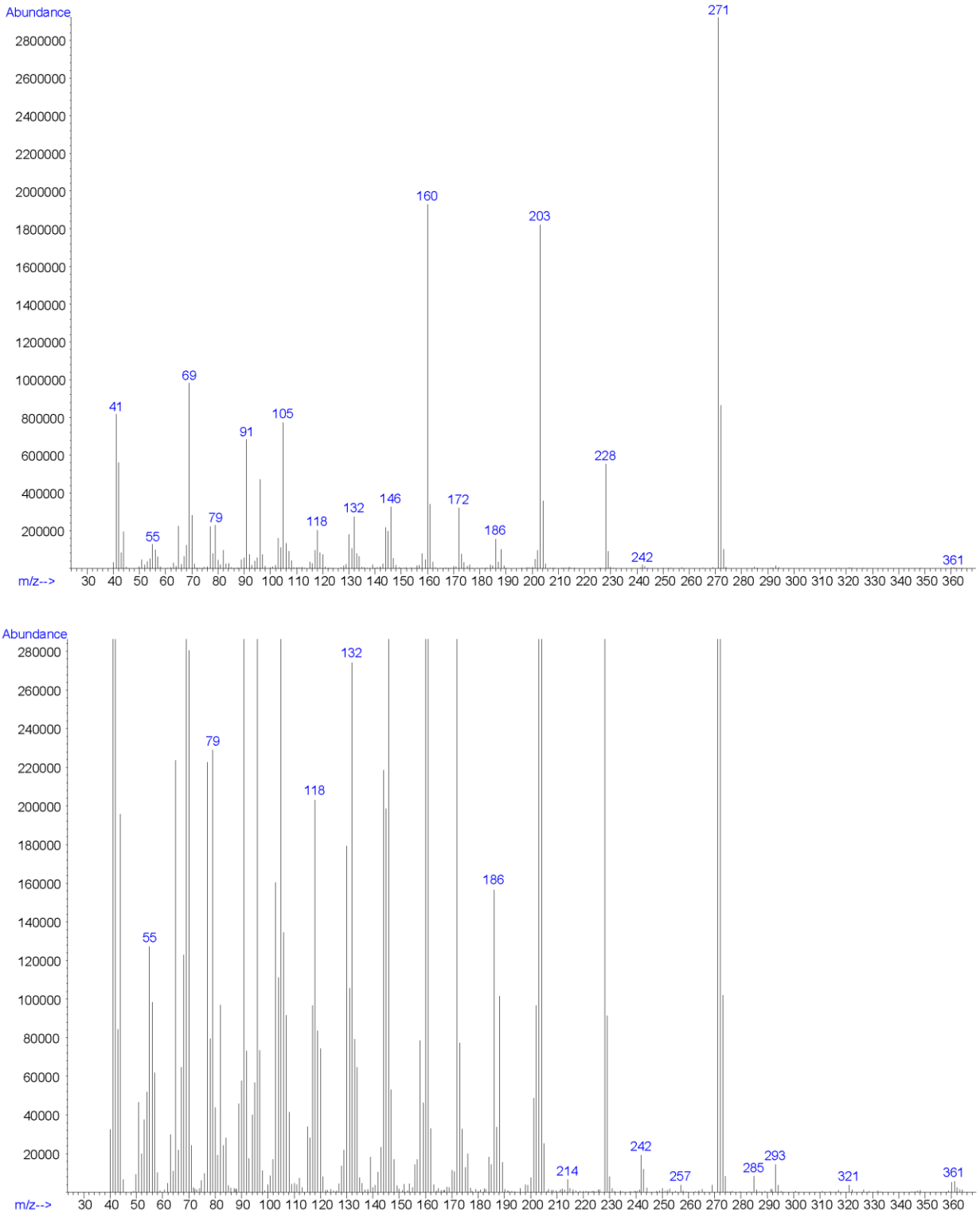
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.254 min
Standard Comparison:	Reference material for *para*-Methylcyclopropylfentanyl (Batch: 0513471-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *para*-Methylcyclopropylfentanyl, based on retention time (8.242 min) and mass spectral data. (https://www.caymanchem.com/product/23045)

Chromatogram: *para*-Methylcyclopropylfentanyl



Additional peaks present in chromatogram: internal standards (3.217 min and 6.287 min)

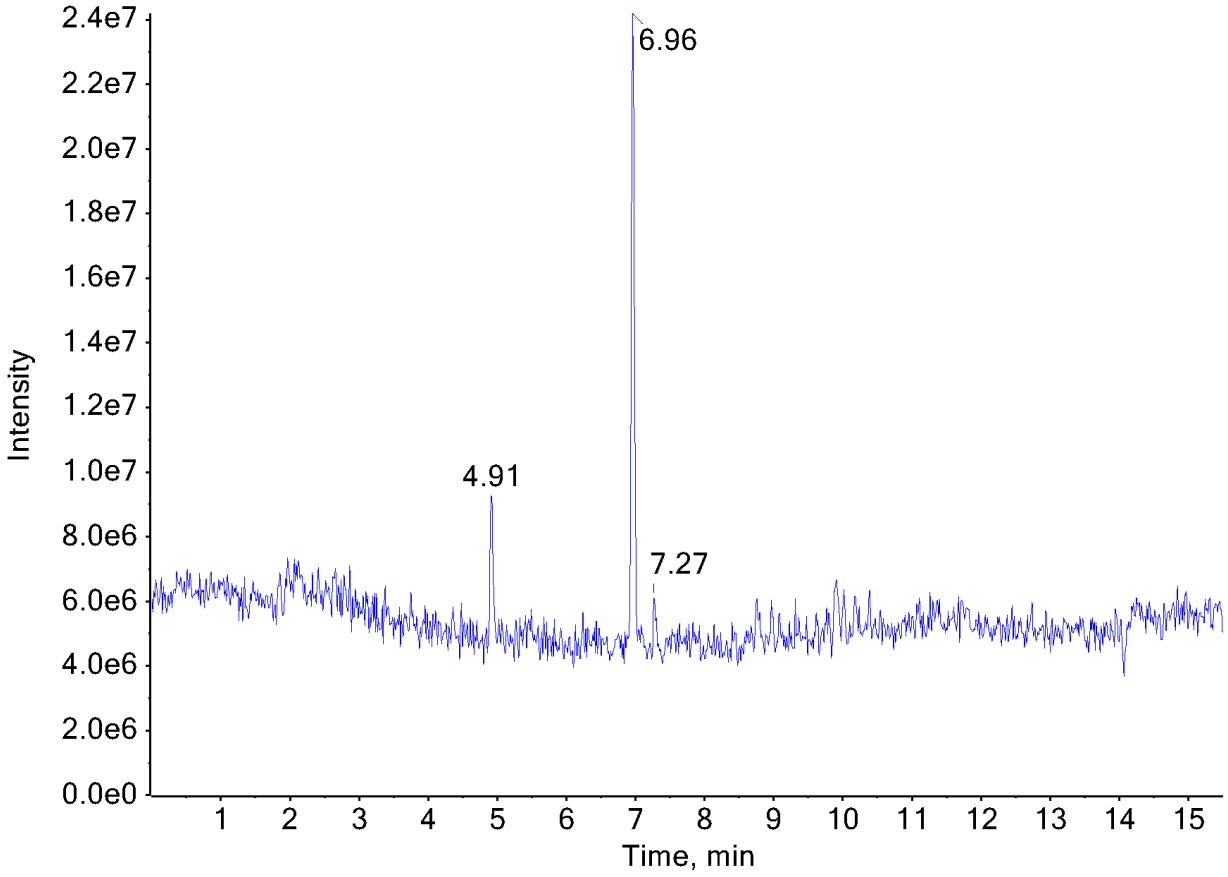
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *para*-Methylcyclopropylfentanyl



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:	6.96 min
Standard Comparison:	Reference material for *para*-Methylcyclopropylfentanyl (Batch: 0513471-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *para*-Methylcyclopropylfentanyl, based on retention time (7.01 min) and mass spectral data. (https://www.caymanchem.com/product/23045)

Chromatogram: *para*-Methylcyclopropylfentanyl



Additional peaks present in chromatogram: internal standards (4.91 min and 7.27 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: *para*-Methylcyclopropylfentanyl