

NMS Labs 2300 Stratford Ave Willow Grove, PA 19090

# **UF-17**



Sample Type: Seized Material

Latest Revision: July 22, 2019 Date Received: May 7, 2019 Date of Report: June 18, 2019

## **1. GENERAL INFORMATION**

IUPAC Name:	N-[2-(dimethylamino)cyclohexyl]-N-phenyl-propanamide	
InChI String:	InChI=1S/C17H26N2O/c1-4-17(20)19(14-10-6-5-7-11-14)16-13- 9-8-12-15(16)18(2)3/h5-7,10-11,15-16H,4,8-9,12-13H2,1-3H3	
CFR:	Not Scheduled (06/2019)	
CAS#	Not Available	
Synonyms:	U-17	
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.

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## 2. CHEMICAL AND PHYSICAL DATA

## 2.1 CHEMICAL DATA

Form	Chemical	Molecular	Molecular Ion	Exact Mass
	Formula	Weight	[M <sup>+</sup> ]	[M+H] <sup>+</sup>
Base	$C_{17}H_{26}N_2O$	274.4	274	275.2118

#### **3. BRIEF DESCRIPTION**

UF-17 is a drug synthetized during pharmaceutical discovery by the Upjohn Company as an antidepressant agent.<sup>1</sup> The "UF-17" name was created by Cayman Chemical due to structural resemblance with U-47700 and fentanyl, two synthetic opioids, as well as the number scheme from its original patent. No information is available regarding the activity or receptor binding profile of UF-17, specifically relating to the opioid receptor system; therefore, this substance has not been assigned a subclassification under the novel psychoactive substance (NPS) class of emerging drugs. Furanyl UF-17 is a structurally similar substance to UF-17. UF-17 and Furanyl UF-17 are not scheduled substances in the United States.

#### 4. ADDITIONAL RESOURCES

 Szmuszkovicz, J; VonVoigtlander, PF; Kane, MP. A New Nontricyclic Antidepressant Agent. Synthesis and Activity of N-[trans-2-(Dimethylamino)cyclopentyl]-N-(3,4dichlorophenyl)propanamide and Related Compounds. *J Med Chem.* 1981, 23, 1230-1236. https://www.ncbi.nlm.nih.gov/pubmed/7328583

https://www.caymanchem.com/product/27925

## **5. QUALITATIVE DATA**

#### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

<b>Testing Performed At:</b>	NMS Labs (Willow Grove, PA)	
Sample Preparation:	Acid/Base extraction	
Instrument:	Agilent 5975 Series GC/MSD System	
Column:	Zebron <sup>TM</sup> Inferno <sup>TM</sup> ZB-35HT (15 m x 250 $\mu$ m x 0.25 $\mu$ m)	
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
<b>Injection Parameters:</b>	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
<b>Retention Time:</b>	5.678 min
Standard Comparison:	Reference material for UF-17 (Batch: 0558710-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as UF-17, based on retention time (5.676 min) and mass spectral data. ( <u>https://www.caymanchem.com/product/27925</u> )

# **Chromatogram: UF-17**



Additional peaks present in chromatogram: internal standards (3.203 min and 6.285 min)



EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): UF-17

# 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	
<b>Injection Parameters:</b>	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	
<b>Retention Time:</b>	5.61 min	
Standard Comparison:	Reference material for UF-17 (Batch: 0558710-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as UF-17, based on retention time (5.59 min) and mass spectral data. (https://www.caymanchem.com/product/27925)	

# Chromatogram: UF-17



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

## TOF MS (Top) and MS/MS (Bottom) Spectra: UF-17



# 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."