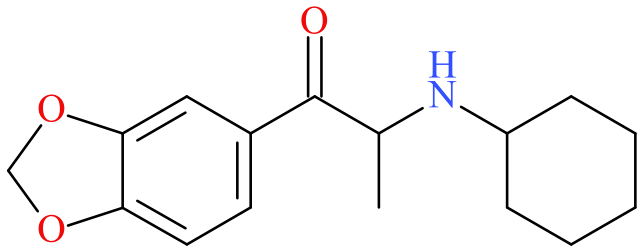
N-Cyclohexyl Methylone

Sample Type: **Drug Material**



Latest Revision: **May 9, 2022**

Date Received: **January 25, 2022**

Date of Report: **May 9, 2022**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(cyclohexylamino)propan-1-one
InChI String:	InChI=1S/C16H21NO3/c1-11(17-13-5-3-2-4-6-13)16(18)12-7-8-14-15(9-12)20-10-19-14/h7-9,11,13,17H,2-6,10H2,1H3
CFR:	Not Scheduled (05/2022)
CAS#	Not Available
Synonyms:	Cyputylone, 3,4-Methylenedioxy-N-Cyclohexylcathinone, 3,4-Methylenedioxy-α-Cyclohexylaminopropiophenone
Source:	(1) Indianapolis-Marion County Forensic Services Agency (2) Miami Dade Police Department
Appearance:	(1) Ecstasy Tablet (2) Beige Crystalline Rock and Off-White Crystalline Powder

***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; Vanquilla Shellman Francis, PhD; Ryan Farrell; Kaitlin Schilde, MSFS; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sara E. Walton, MS; 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	$C_{16}H_{21}NO_3$	275.3	275	276.1594

3. BRIEF DESCRIPTION

N-Cyclohexyl methylone 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 psychoactive effects similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar drugs include methylone and diethlyone (or *N*,*N*-diethyl methylone), among other *beta*-keto methylenedioxyamphetamine (or "-ylones"). Methylone is a Schedule I substance in the United States; *N*-cyclohexyl methylone is not explicitly scheduled.

N-Cyclohexyl methylone has been mentioned in online drug forums and appeared for sale on surface web gray market vendor sites under the name "cyputylone". Scientific experts agree that the name "cyputylone" is not preferred due to nomenclature inconsistency and potential for confusion, and rather suggest the name "*N*-cyclohexyl methylone" be universally used instead.

4. ADDITIONAL RESOURCES

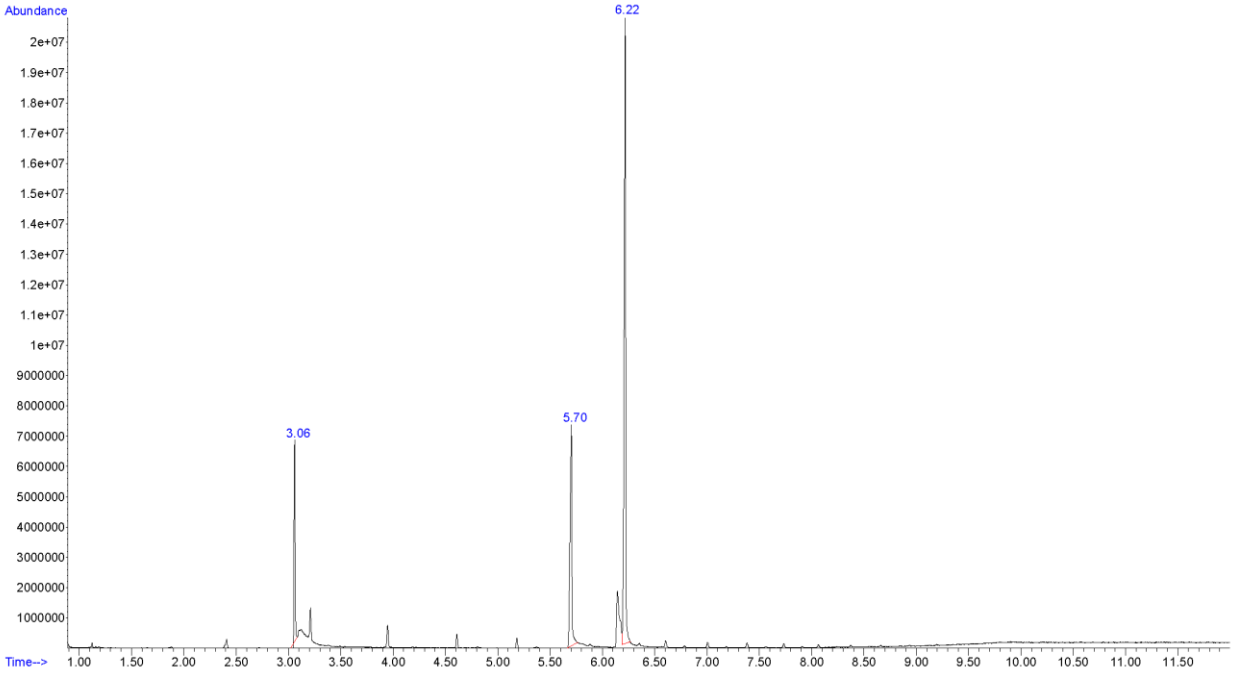
https://www.caymanchem.com/product/35165/3%2C4-methylenedioxy-%CE%B1-cyclohexylaminopropiophenone-(hydrochloride)

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

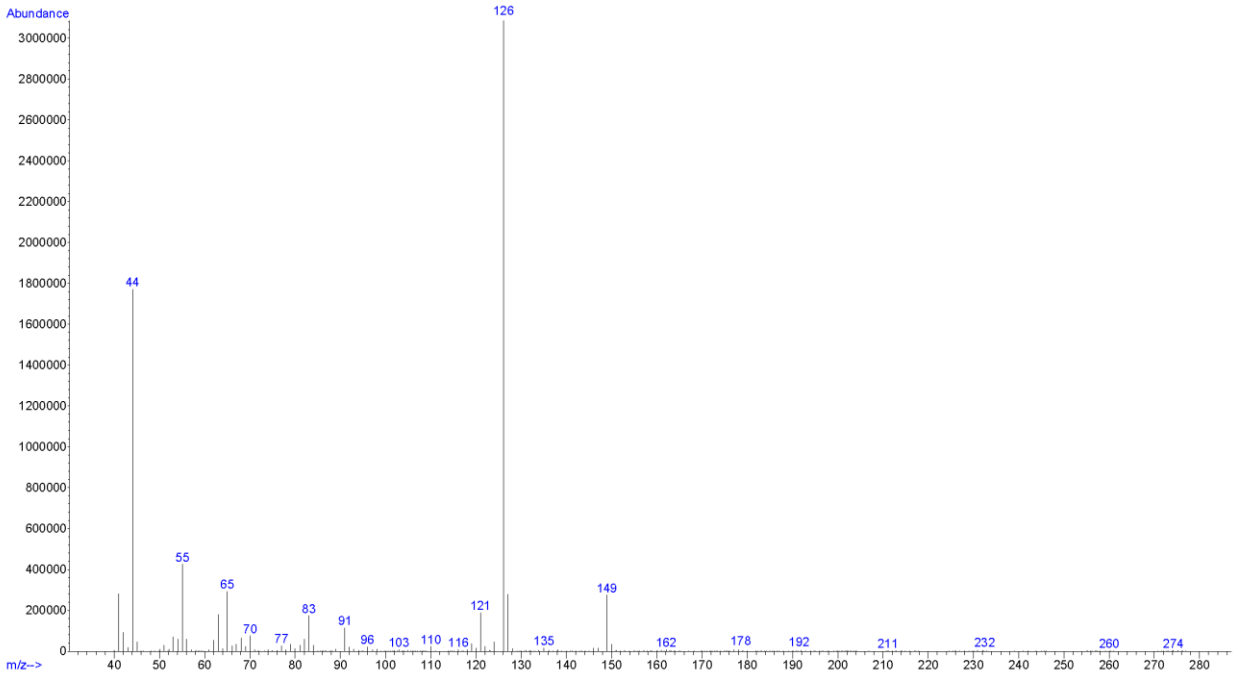
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Miami Dade Police Department)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: 1.46 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.22 min
Standard Comparison:	Reference material for *N*-Cyclohexyl Methylone (Batch: 0628328-6) 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*-Cyclohexyl Methylone based on retention time (6.20 min) and mass spectral data. (https://www.caymanchem.com/product/35165/3%2C4-methylenedioxy-%CE%B1-cyclohexylaminopropiophenone-(hydrochloride))

Chromatogram: *N*-Cyclohexyl Methylone



Additional peaks in chromatogram: internal standards (3.06 and 5.70 mins)

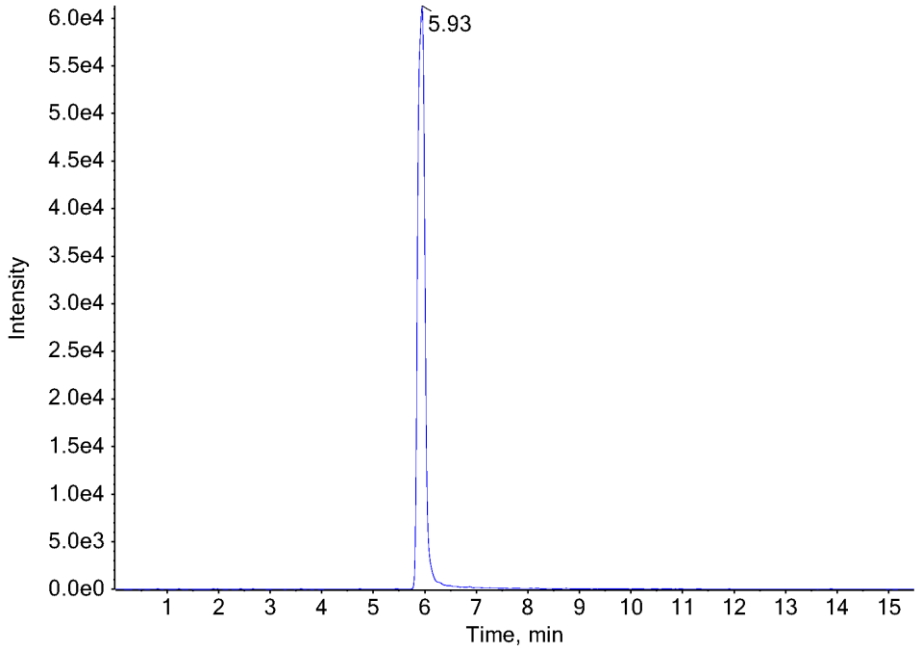
EI (70 eV) Mass Spectrum: *N*-Cyclohexyl Methylone



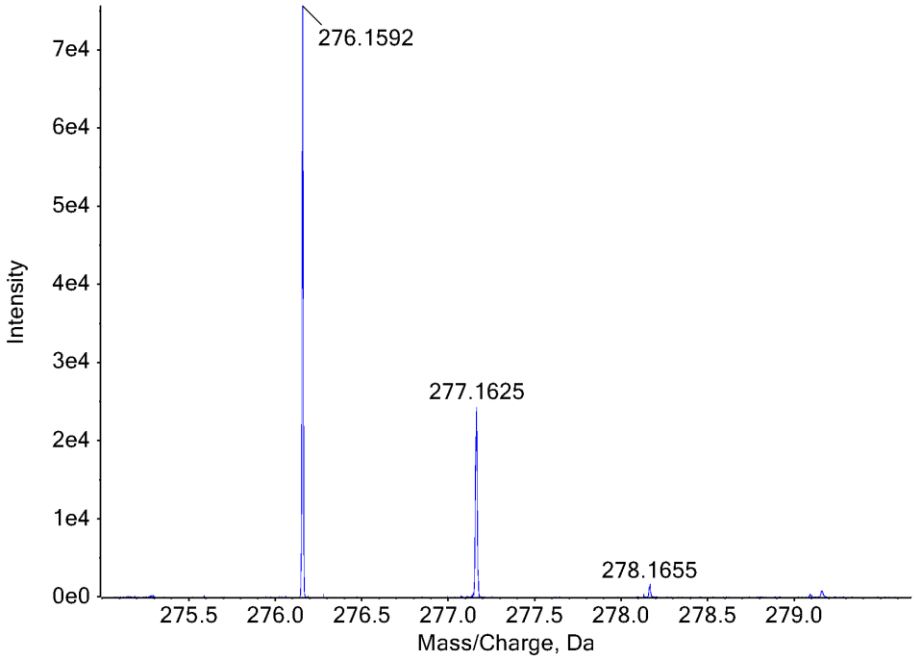
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Miami Dade Police Department) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
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:	5.93 min
Standard Comparison:	Reference material for *N*-Cyclohexyl Methylone (Batch: 0628328-6) 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*-Cyclohexyl Methylone based on retention time (5.84 min) and mass spectral data. (https://www.caymanchem.com/product/35165/3%2C4-methylenedioxy-%CE%B1-cyclohexylaminopropiophenone-(hydrochloride))

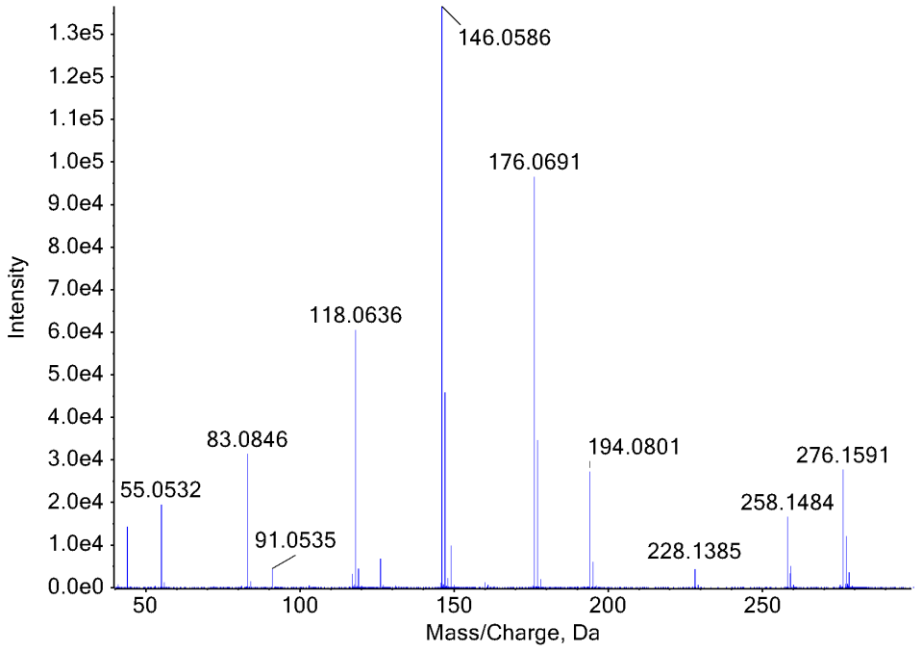
Extracted Ion Chromatogram: *N*-Cyclohexyl Methylone



TOF MS Spectra: *N*-Cyclohexyl Methylone



TOF MS/MS Spectra: *N*-Cyclohexyl Methylone



6. FUNDING

NPS Discovery at the Center for Forensic Science Research and Education (CFSRE) is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, "Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)"). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the Department of Justice.