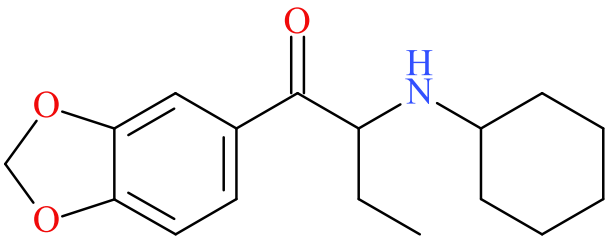
N-Cyclohexyl Butylone

Sample Type: **Drug Material**



Latest Revision: **June 9, 2022**

Date Received: **February 17, 2022**

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

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(cyclohexylamino)butan-1-one
InChI String:	InChI=1S/C17H23NO3/c1-2-14(18-13-6-4-3-5-7-13)17(19)12-8-9-15-16(10-12)21-11-20-15/h8-10,13-14,18H,2-7,11H2,1H3
CFR:	Not Scheduled (06/2022)
CAS#	Not Available
Synonyms:	Cybutylone 3,4-Methylenedioxy-α-Cyclohexylaminobutiophenone
Source:	(1) Indianapolis-Marion County Forensic Services Agency (2) Miami Dade Police Department
Appearance:	(1) Plant-Like Material *(Data not included; sample also contained CH-PIATA, N,N-dimethylpentylone, and N-cyclohexyl methylone)* (2) White Crystalline Powder, Beige Powder and Rocks

***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.*

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{17}H_{23}NO_3$	289.4	289	290.1751

3. BRIEF DESCRIPTION

N-Cyclohexyl butylone 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 *N*-cyclohexyl methylone (reported by NPS Discovery in May 2022) and butylone, among other *beta*-keto methylenedioxyamphetamine (or "-ylones"). Butylone is a Schedule I substance in the United States; *N*-cyclohexyl butylone and *N*-cyclohexyl methylone are not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/36884/n-cyclohexyl-butylone-(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)

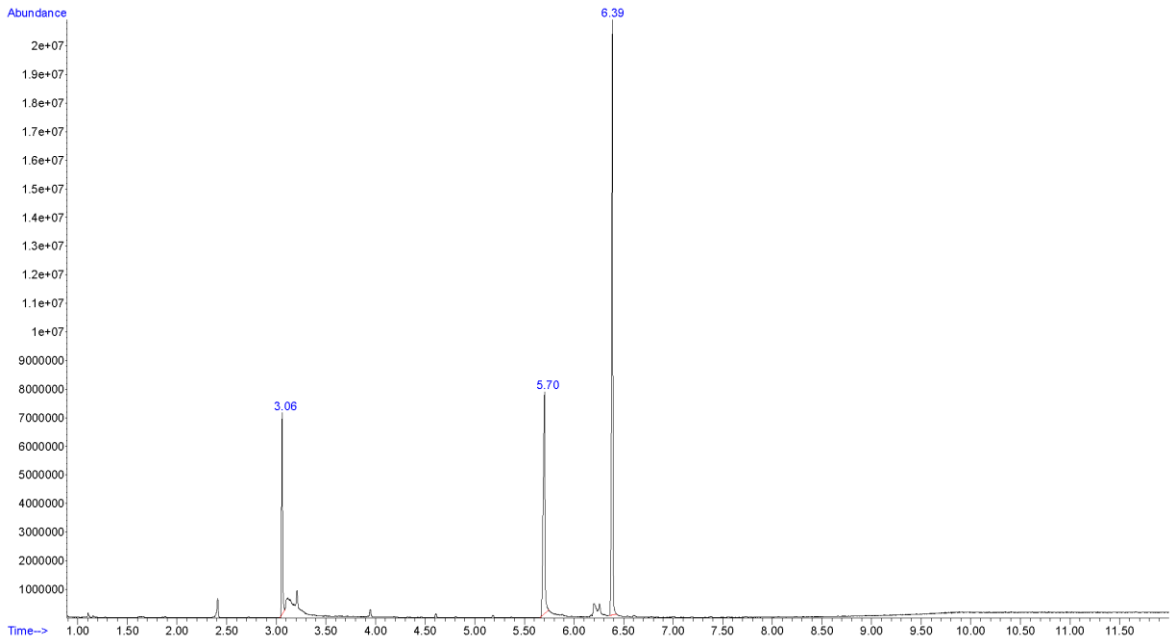
Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

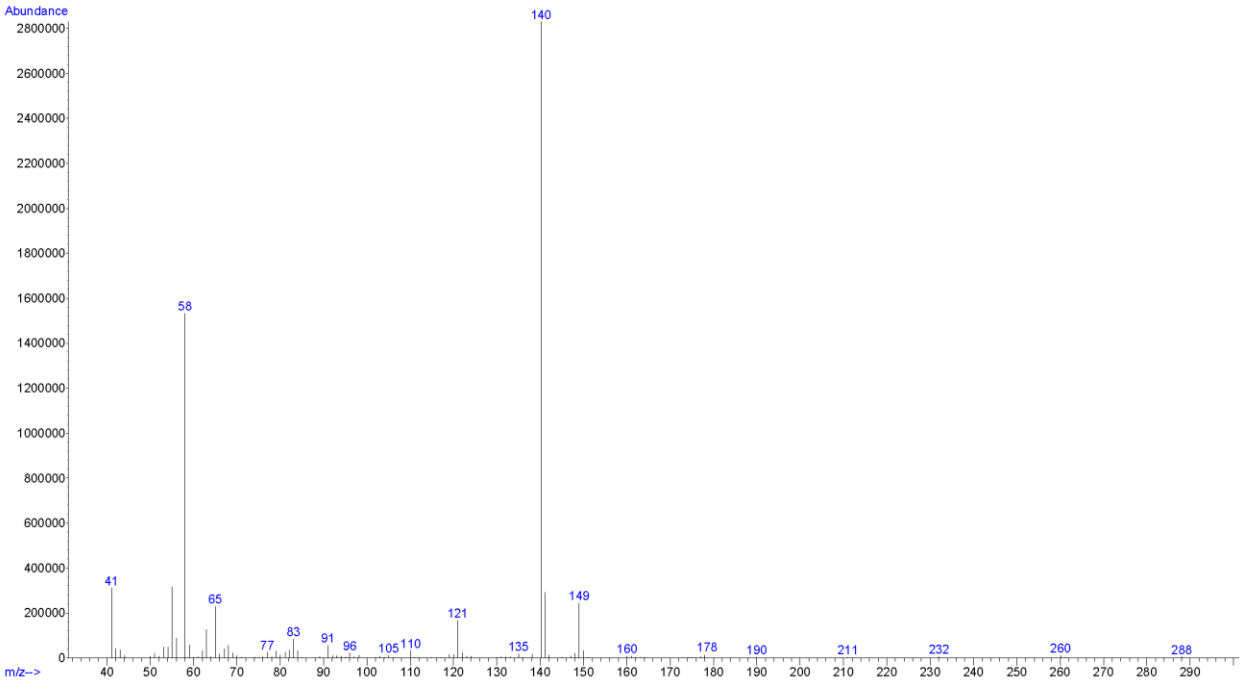
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.39 min
Standard Comparison:	Reference material for *N*-Cyclohexyl Butylone (Batch: 0646340-2) 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 Butylone based on retention time (6.43 min) and mass spectral data. (https://www.caymanchem.com/product/36884/n-cyclohexyl-butylone-(hydrochloride))

Chromatogram: *N*-Cyclohexyl Butylone



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

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

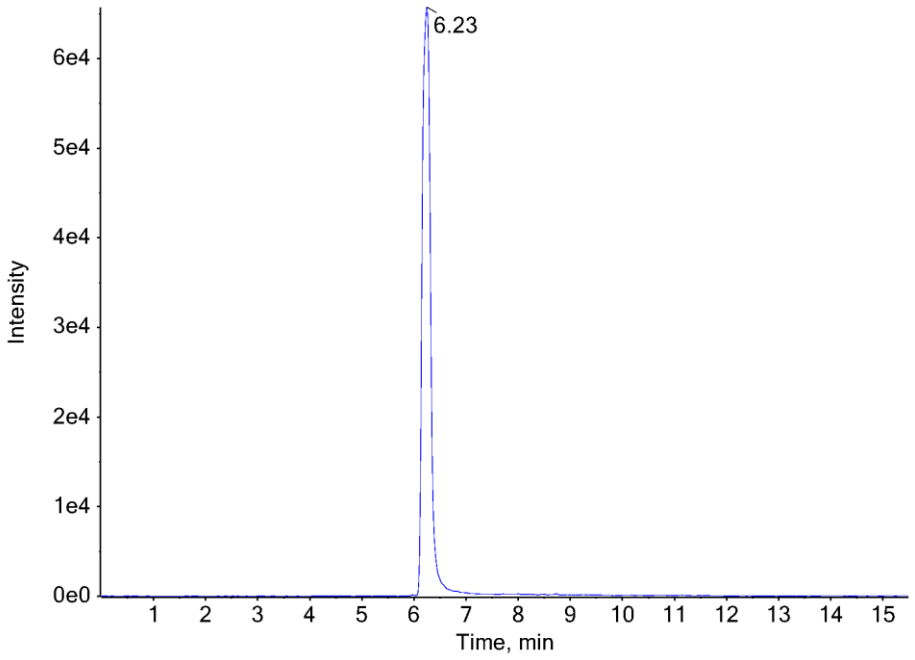


5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

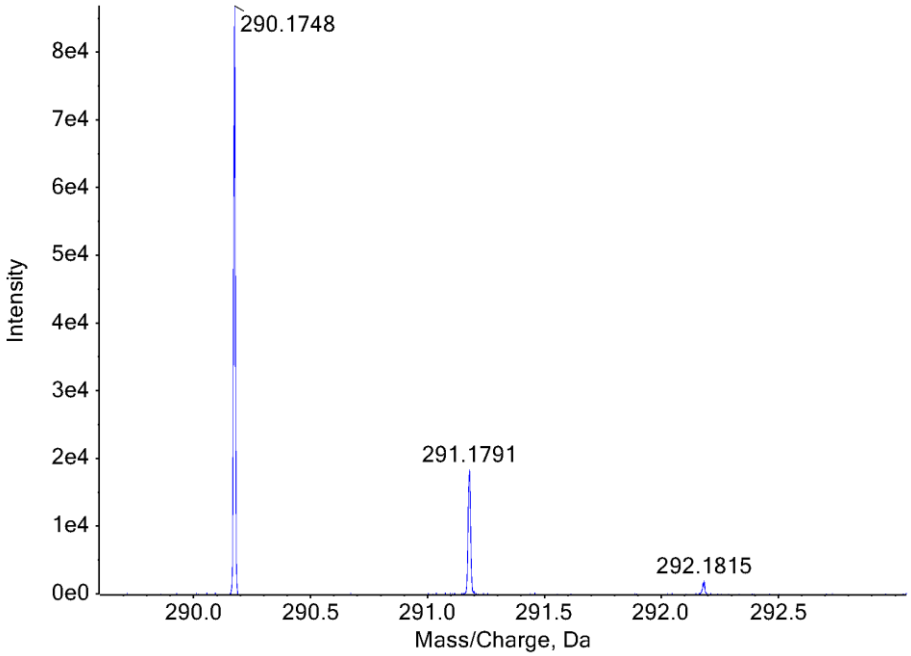
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Miami Dade Police Department) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
Instrument:	Sciex TripleTOF® 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:	6.23 min
Standard Comparison:	Reference material for *N*-Cyclohexyl Butylone (Batch: 0646340-2) 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 Butylone based on retention time (6.20 min) and mass spectral data. (https://www.caymanchem.com/product/36884/n-cyclohexyl-butylone-(hydrochloride))

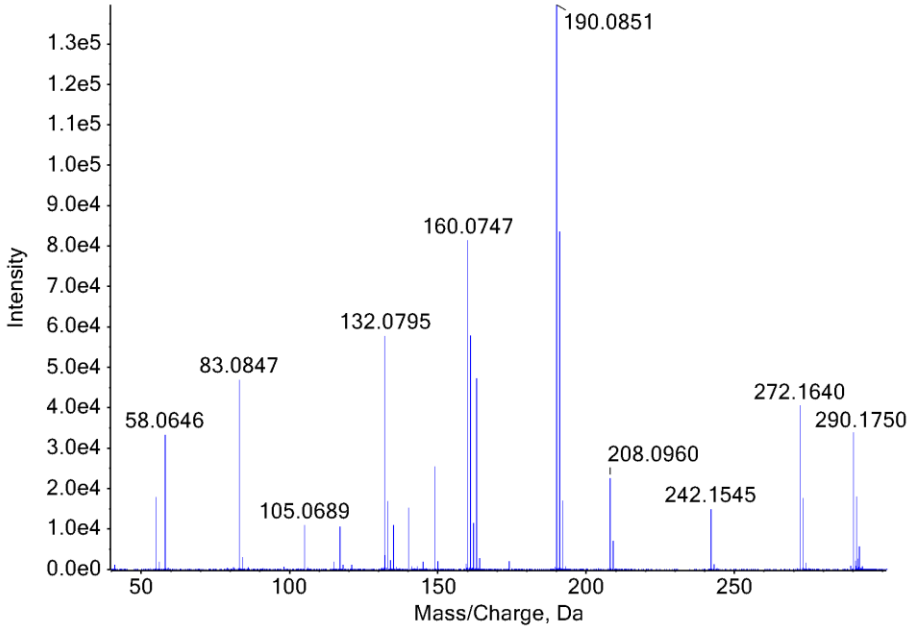
Extracted Ion Chromatogram: *N*-Cyclohexyl Butylone



TOF MS Spectra: *N*-Cyclohexyl Butylone



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



6. FUNDING

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