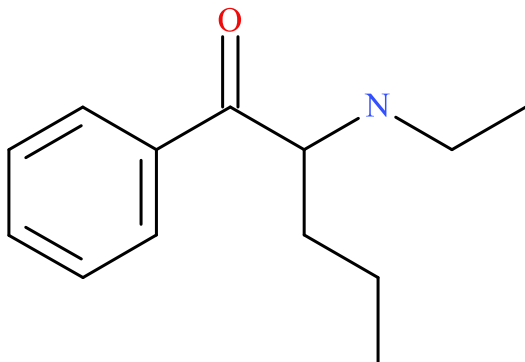# *N*-Ethyl Pentedrone

Sample Type: **Biological Fluid**

Latest Revision: **February 24, 2020**

Date of Report: **February 24, 2020**

1. GENERAL INFORMATION

IUPAC Name: 2-(ethylamino)-1-phenyl-pentan-1-one

InChI String: InChI=1S/C13H19NO/c1-3-8-12(14-4-2)13(15)11-9-6-5-7-10-11/h5-7,9-10,12,14H,3-4,8H2,1-2H3

CFR: Not Scheduled (02/2020)

CAS#   18268-16-1

Synonyms: α-Ethylaminopentiophenone

Source: NMS Labs – Toxicology Department

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M⁺]	Exact Mass [M+H]⁺
N-Ethyl Pentedrone	$C_{13}H_{19}NO$	205.3	205	206.1539

Important Note: *All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.*

Report Prepared By: *Alex J. Krotulski, PhD, and Barry K. Logan, PhD, F-ABFT*

3. SAMPLE HISTORY

N-Ethyl pentedrone has been identified in three cases. The geographical and demographical breakdown is below:

Geographical Location: Indiana (n=1), Minnesota (n=1), California (n=1)

Biological Sample: Blood (n=3), Urine (n=1)

Date of First Receipt: September 28, 2019

Other Notable Findings: Eutylone, 4F-Methylphenidate, Flualprazolam, Etizolam, and Methamphetamine

4. BRIEF DESCRIPTION

N-Ethyl pentedrone 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 stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include pentedrone, 4F-pentedrone, hexedrone, and *N*-ethyl hexedrone. Pentedrone is a Schedule I substance in the United States while *N*-ethyl pentedrone is not explicitly scheduled.

5. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/14280/

6. QUALITATIVE DATA

6.1 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: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for *N*-ethyl pentedrone (Batch: 0446282-31) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/14280/)

EI (70 eV) Mass Spectrum: *N*-Ethyl Pentedrone (Standard)
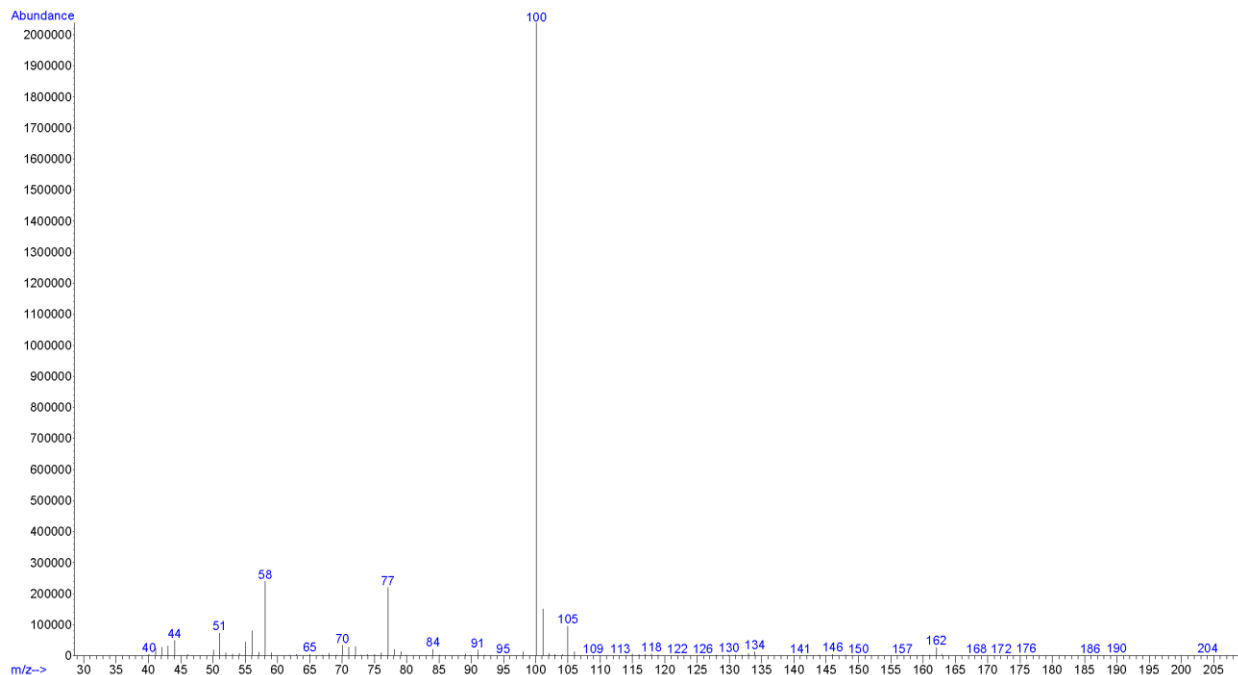
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: No additional preparation - direct analysis of sample extract

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

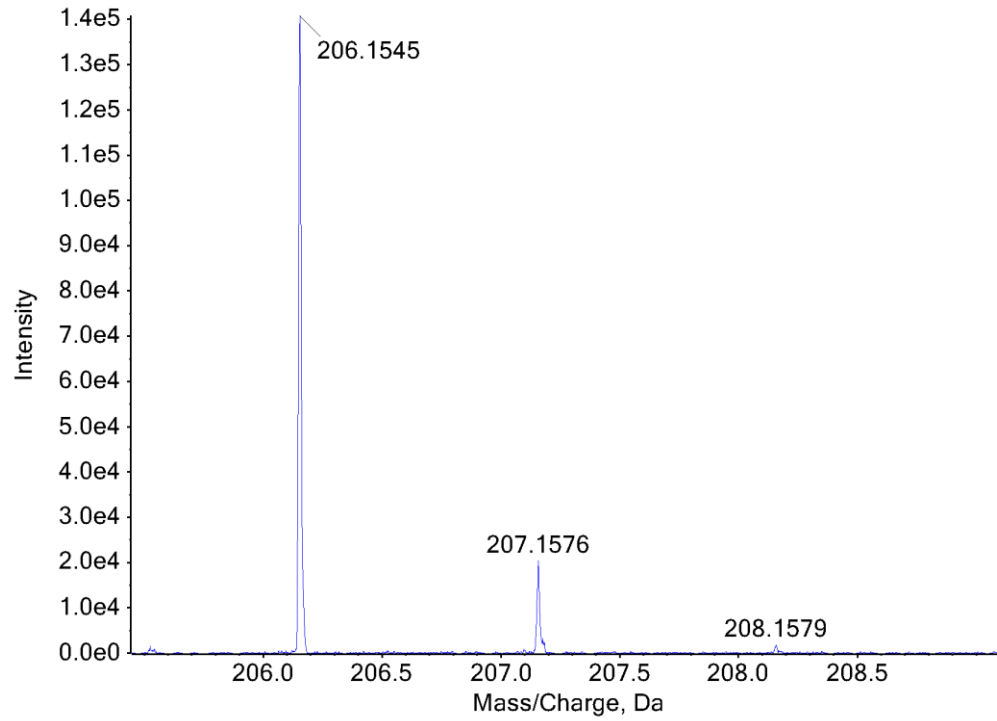|	
Gradient:	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	5.05 min
Standard Comparison:	Reference material for *N*-ethyl pentedrone (Batch: 0446282-31) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as *N*-ethyl pentedrone, based on retention time (5.06 min) and mass spectral data. (https://www.caymanchem.com/product/14280/)

Extracted Ion Chromatogram: *N*-Ethyl Pentedrone
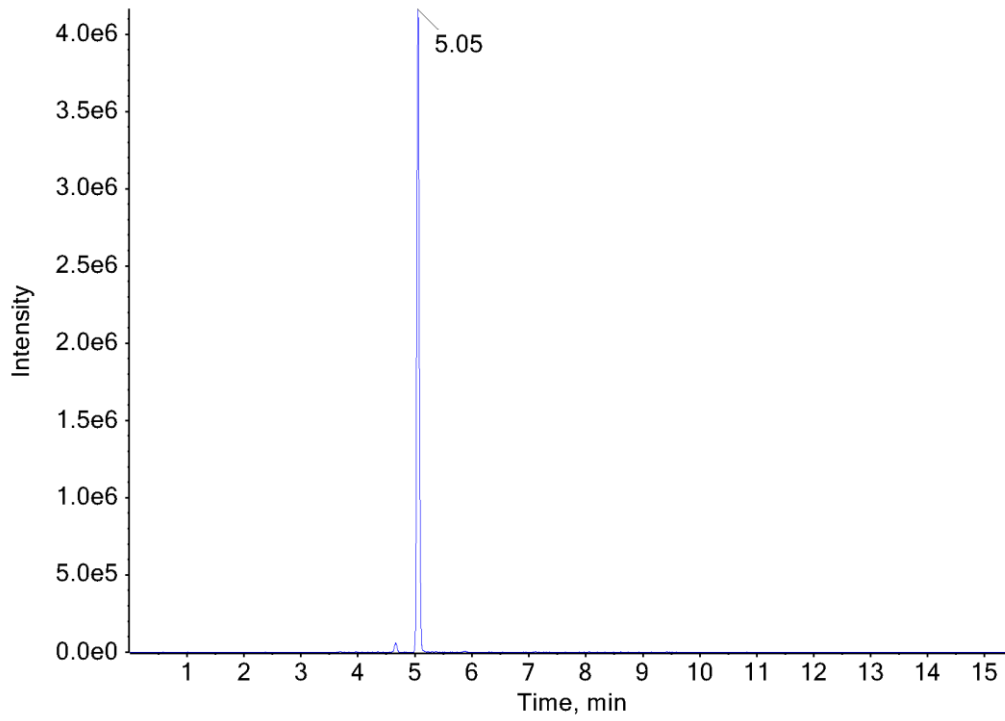
TOF MS Spectrum: *N*-Ethyl Pentedrone

MS/MS Spectrum: *N*-Ethyl Pentedrone