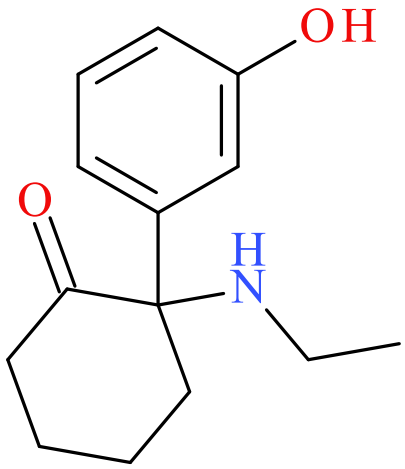
Hydroxetamine (HXE)

Sample Type: **Toxicology Sample**



Latest Revision: **August 31, 2022**

Date Received: **November 16, 2021**

Date of Report: **August 31, 2022**

1. GENERAL INFORMATION

IUPAC Name:	2-(ethylamino)-2-(3-hydroxyphenyl)cyclohexanone
InChI String:	InChI=1S/C14H19NO2/c1-2-15-14(9-4-3-8-13(14)17)11-6-5-7-12(16)10-11/h5-7,10,15-16H,2-4,8-9H2,1H3
CFR:	Not Scheduled (05/2022)
CAS#	1620054-73-0
Synonyms:	HXE, O-desmethyl Methoxetamine, 3-hydroxy-2-oxo-PCE
Source:	NMS Labs – Toxicology Department

***Important Note**: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The "3-hydroxy" configuration was used for structural purposes; however, position of the hydroxy group was not confirmed during analysis.*

***Prepared By:** Alex J. Krotulski, PhD; Sara E. Walton, MS; Melissa F. Fogarty, MSFS, D-ABFT-FT; Donna M. Papsun, MS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Hydroxetamine	$C_{14}H_{19}NO_2$	233.3	233	234.1489

3. SAMPLE HISTORY

Hydroxetamine has been identified in at least one toxicology case since November 2021. The geographical and demographical breakdown is below:

Case Type: Postmortem (n=1)

Geographical Location: Canada (n=1)

Biological Sample: Peripheral Blood (n=1)

Date of First Collection: November 2021

Additional NPS Findings: Methoxetamine (MXE) *[peak area much smaller than HXE]*, Ketamine, Etizolam, Mitragynine, Brorphine

4. BRIEF DESCRIPTION

Hydroxetamine (HXE) is classified as a novel hallucinogen. Novel hallucinogens have been reported to cause effects similar to ketamine and phencyclidine (PCP). Novel hallucinogens have been linked to adverse events, including deaths, as described in the literature. Structurally similar drugs include methoxetamine (MXE), deschloro-*N*-ethyl ketamine (O-PCE), and other similar analogues. Hydroxetamine and methoxetamine are not explicitly scheduled substances in the United States.

5. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/HXE-ID-2266-21_reportfin.pdf

https://www.caymanchem.com/product/33774/hydroxetamine

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

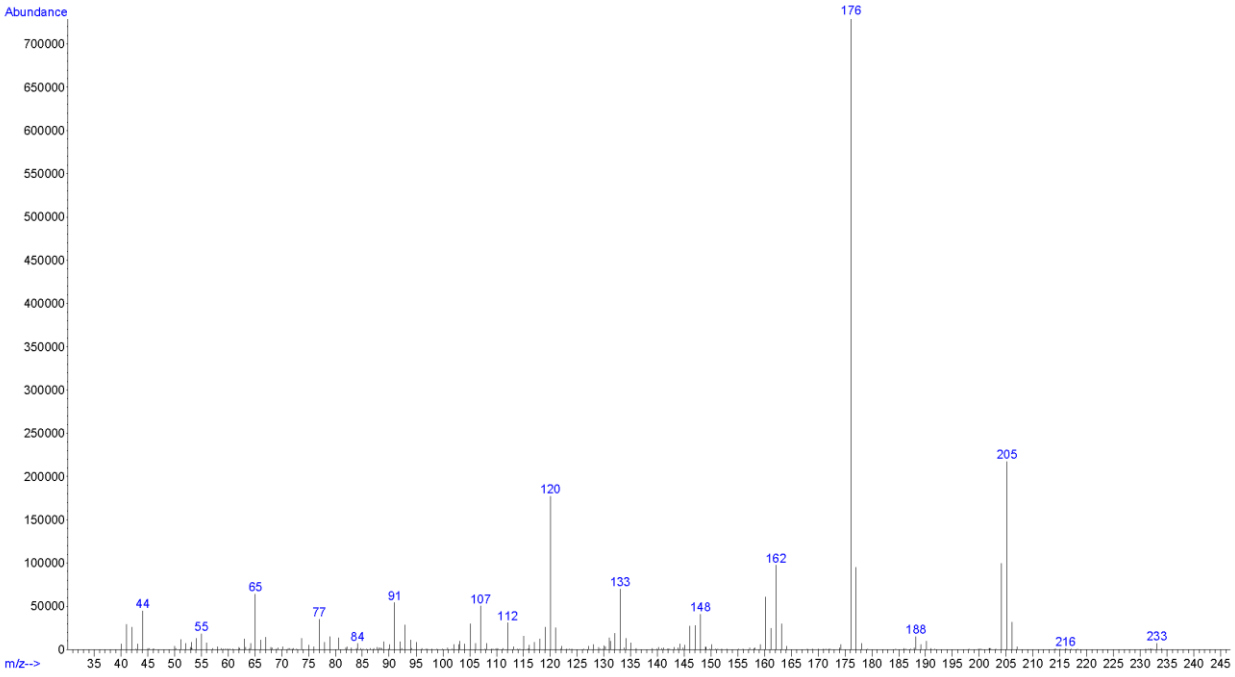
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for hydroxetamine (Batch: 0618566-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/33774/hydroxetamine)

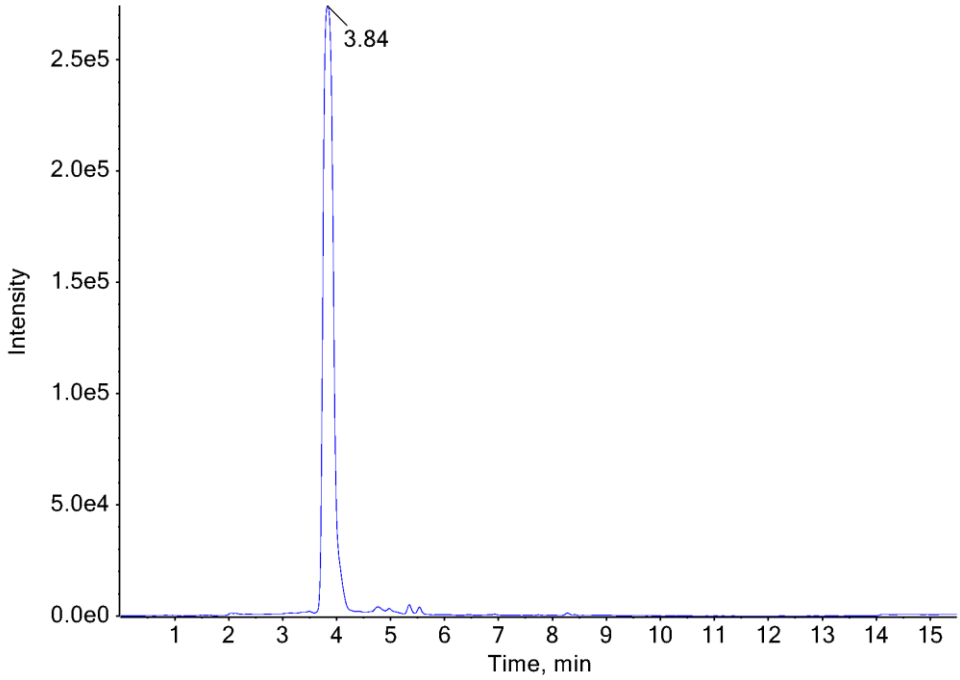
EI (70 eV) Mass Spectrum: Hydroxetamine (Standard)



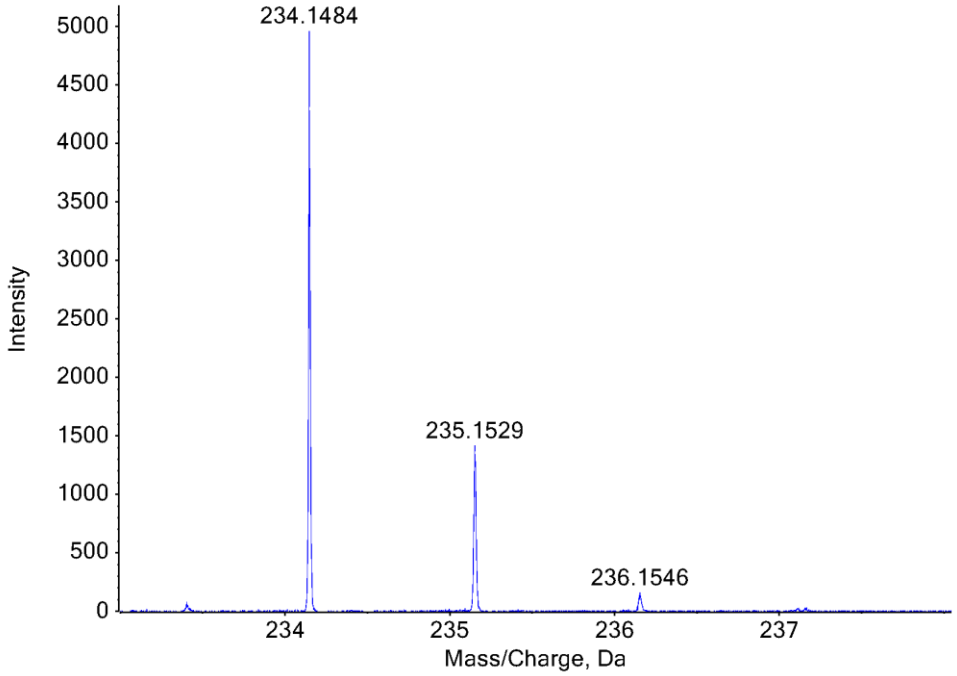
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Liquid-liquid extraction (LLE)
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:	3.84 min
Standard Comparison:	Reference material for hydroxetamine (Batch: 0618566-1) 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 hydroxetamine, based on retention time (4.00 min) and mass spectral data. (https://www.caymanchem.com/product/33774/hydroxetamine)

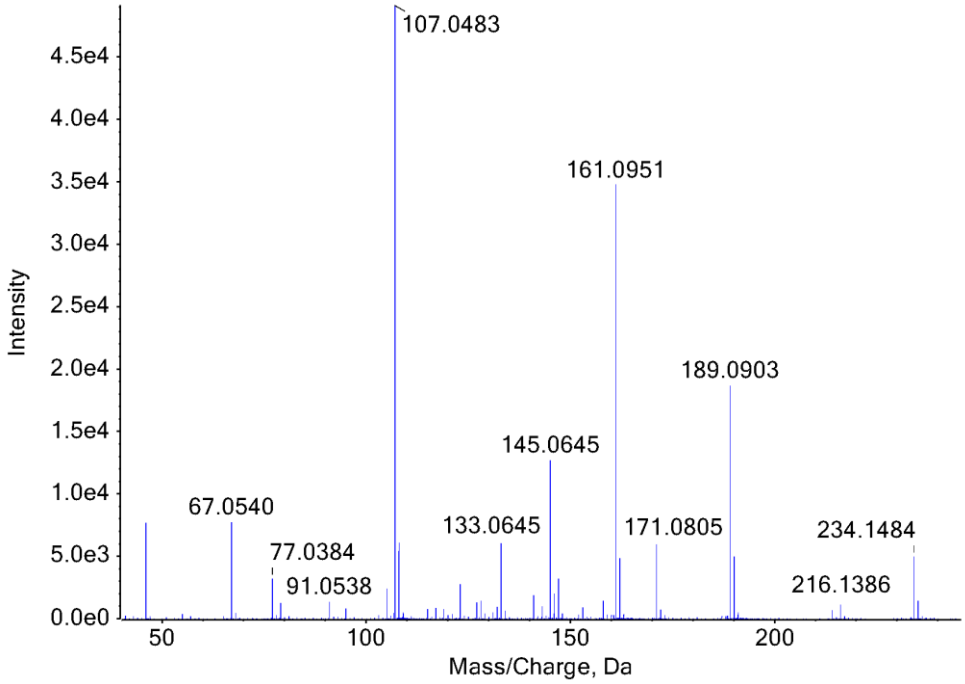
Extracted Ion Chromatogram: Hydroxetamine



TOF MS Spectra: Hydroxetamine



MS/MS Spectra: Hydroxetamine



7. FUNDING

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