

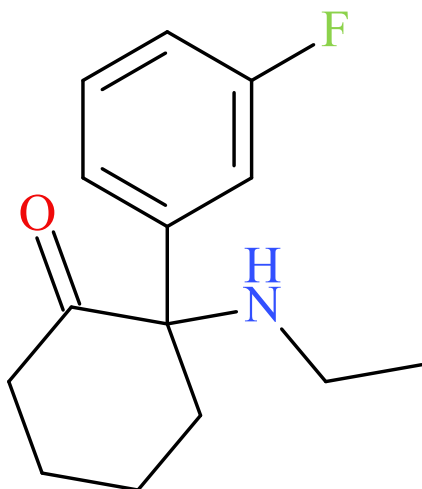
Fluorexetamine (FXE)

Sample Type: **Toxicology Sample**

Latest Revision: **December 16, 2022**

Date Received: **October 31, 2022**

Date of Report: **December 16, 2022**



1. GENERAL INFORMATION

| | |
|----------------------|---|
| IUPAC Name: | 2-(ethylamino)-2-(3-fluorophenyl)cyclohexanone |
| InChI String: | InChI=1S/C14H18FNO/c1-2-16-14(9-4-3-8-13(14)17)11-6-5-7-12(15)10-11/h5-7,10,16H,2-4,8-9H2,1H3 |
| CFR: | Not Scheduled (12/2022) |
| CAS# | Not Available |
| Synonyms: | FXE |
| 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-fluoro” configuration was used for structural purposes; however, position of the fluorine atom was not confirmed during analysis.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

| Drug | Chemical Formula | Molecular Weight | Molecular Ion [M ⁺] | Exact Mass [M+H] ⁺ |
|----------------|-------------------------------------|------------------|---------------------------------|-------------------------------|
| Fluorexetamine | C ₁₄ H ₁₈ FNO | 235.3 | 235 | 236.1445 |

3. SAMPLE HISTORY

Fluorexetamine has been identified in at least one toxicology case since November 2022. The geographical and demographical breakdown is below:

| | |
|----------------------------------|-----------------------------------|
| Case Type: | Postmortem (n=1) |
| Geographical Location: | Ohio (n=1) |
| Biological Sample: | Blood, Urine, and Vitreous (n=1) |
| Date of First Collection: | October 2022 |
| Additional NPS Findings: | Trifluoromethyl-U-47700, Etizolam |

4. BRIEF DESCRIPTION

Fluorexetamine (FXE) 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 hydroxetamine (HXE), methoxetamine (MXE), deschloro-*N*-ethyl ketamine (O-PCE), and other similar analogues. Fluorexetamine, 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/Fluorexetamine-ID-3048-22_report.pdf

[https://www.caymanchem.com/product/35118/fluorexetamine-\(hydrochloride\)](https://www.caymanchem.com/product/35118/fluorexetamine-(hydrochloride))

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

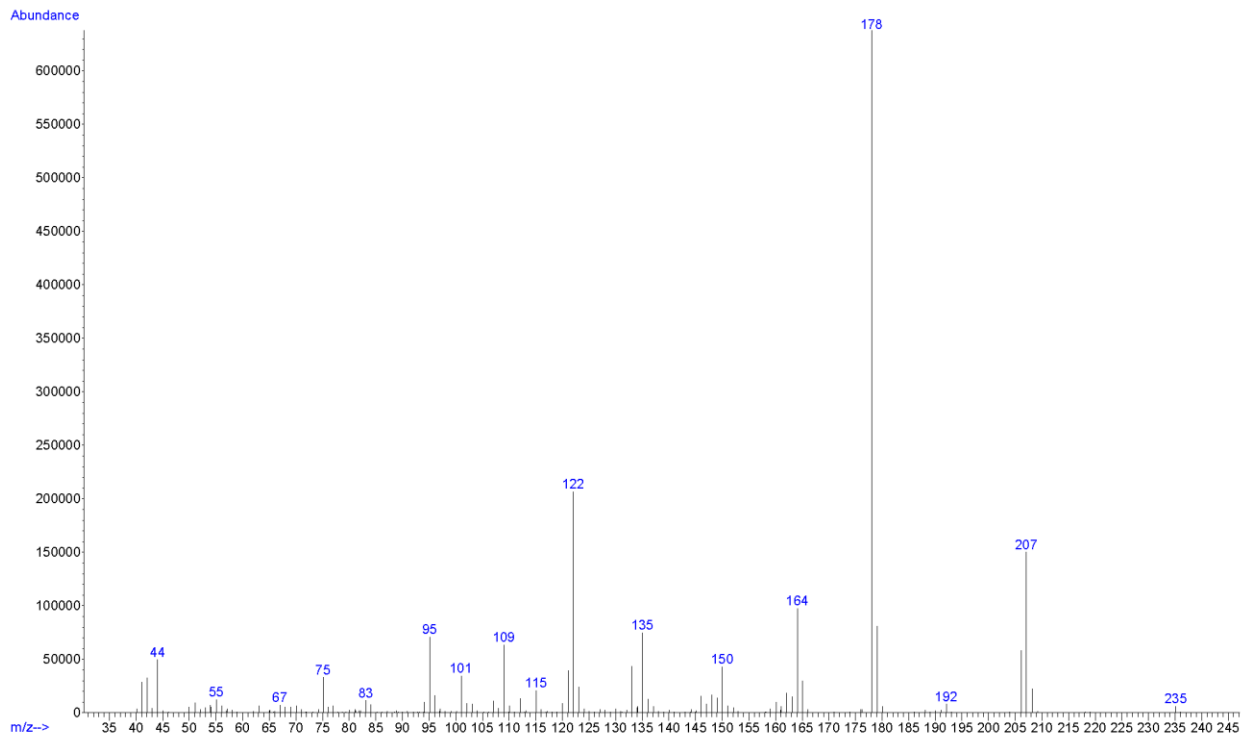
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for fluorexetamine (Batch: 0625438-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA).
(<https://www.caymanchem.com/product/35118/fluorexetamine-hydrochloride>)

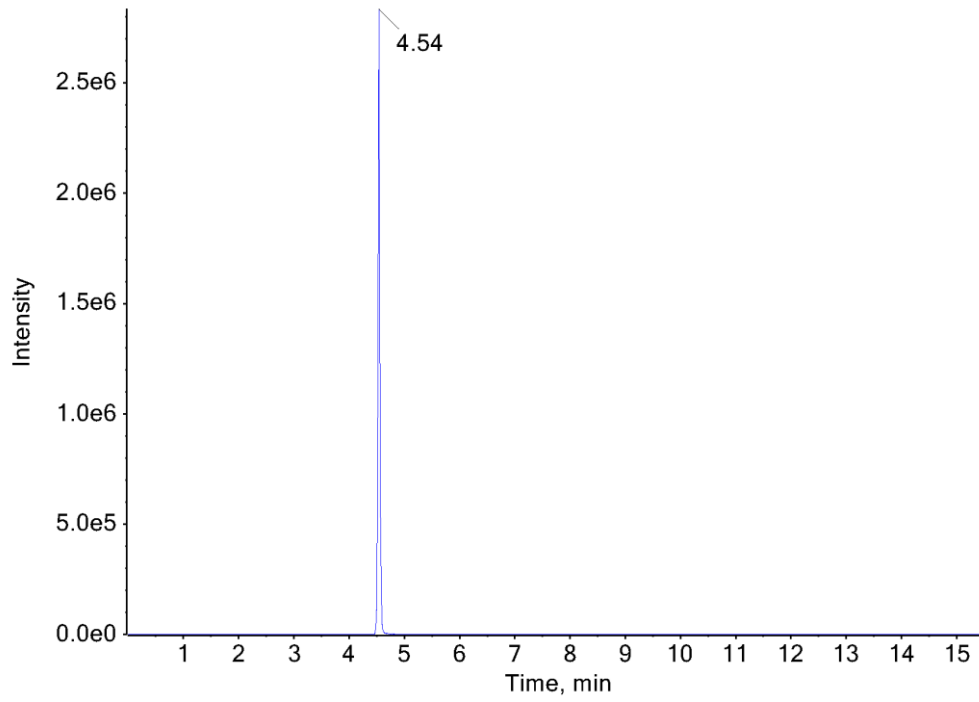
EI (70 eV) Mass Spectrum: Fluorexetamine (Standard)



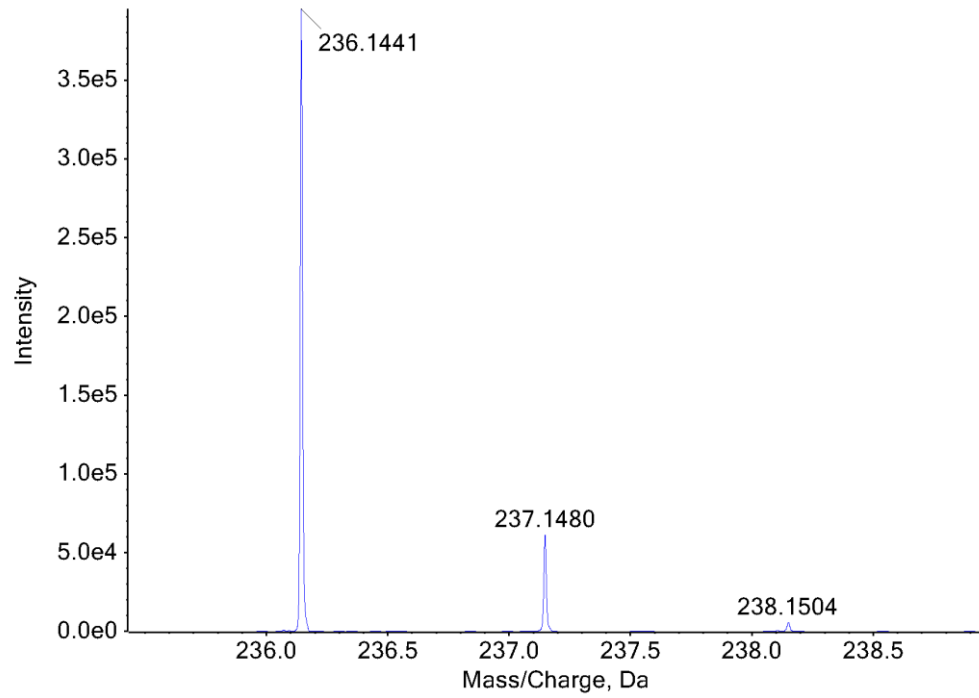
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

| | |
|------------------------------|--|
| 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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da |
| Retention Time: | 4.54 min |
| Standard Comparison: | Reference material for fluorexetamine (Batch: 0625438-1) 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 fluorexetamine, based on retention time (4.63 min) and mass spectral data. https://www.caymanchem.com/product/35118/fluorexetamine-(hydrochloride) |

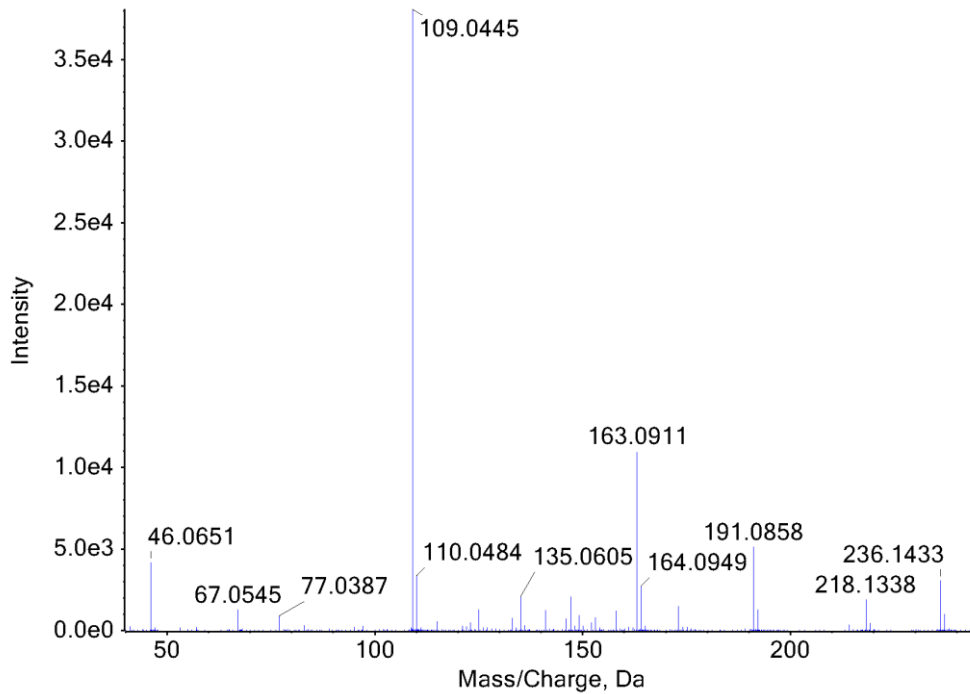
Extracted Ion Chromatogram: Fluorexetamine



TOF MS Spectra: Fluorexetamine



MS/MS Spectra: Fluorexetamine



7. FUNDING

NPS Discovery at the 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 represent the official position or policies of the U.S. Department of Justice.