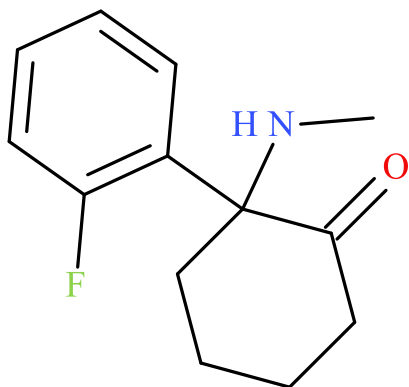


2F-Deschloroketamine

Sample Type: **Biological Fluid**



Latest Revision: **September 4, 2018**

Date of Report: **September 4, 2018**

1. GENERAL INFORMATION

IUPAC Name:	2-(2-fluorophenyl)-2-(methylamino)cyclohexanone
InChI String:	InChI=1S/C13H16FNO/c1-15-13(9-5-4-8-12(13)16)10-6-2-3-7-11(10)14/h2-3,6-7,15H,4-5,8-9H2,1H3
CFR:	Not Scheduled (09/2018)
CAS#	111982-50-4
Synonyms:	2-FDCK, 2-FI-2'-Oxo-PCM, 2-Fluorodeschloroketamine, Fluoroketamine, 2-Fluroketamine, 2-FK, 2F-Ketamine
Source:	NMS Labs – Toxicology Department

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass [M+H] ⁺
2F-Deschloroketamine	C ₁₃ H ₁₆ FNO	221.27	222.1289

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

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

3. SAMPLE HISTORY

2F-Deschloroketamine has been identified in one case since August 2018. The geographical and demographic breakdown is below:

Geographical Location:	Massachusetts
Biological Sample:	Femoral Blood
Date of First Collection:	Not Available
Date of First Receipt:	August 10, 2018
Additional NPS:	MeO-PCP, Etizolam

4. BRIEF DESCRIPTION

2F-Deschloroketamine is classified as a novel dissociative and ketamine analogue. Ketamine analogues are modified based on the structure of ketamine. Ketamine analogues have been reported to cause dissociative, anesthetic, and hallucinogenic effects, similar to ketamine and other dissociative or hallucinogenic agents. Ketamine analogues are not well described in the literature. Ketamine is a Schedule III substance in the United States.

5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/19786>

<https://pubchem.ncbi.nlm.nih.gov/compound/13771618#section=Top>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/2F-ketamine-ID-1818-17_report.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/2-fluoro%20Deschloroketamine-ID-1847-17_report.pdf

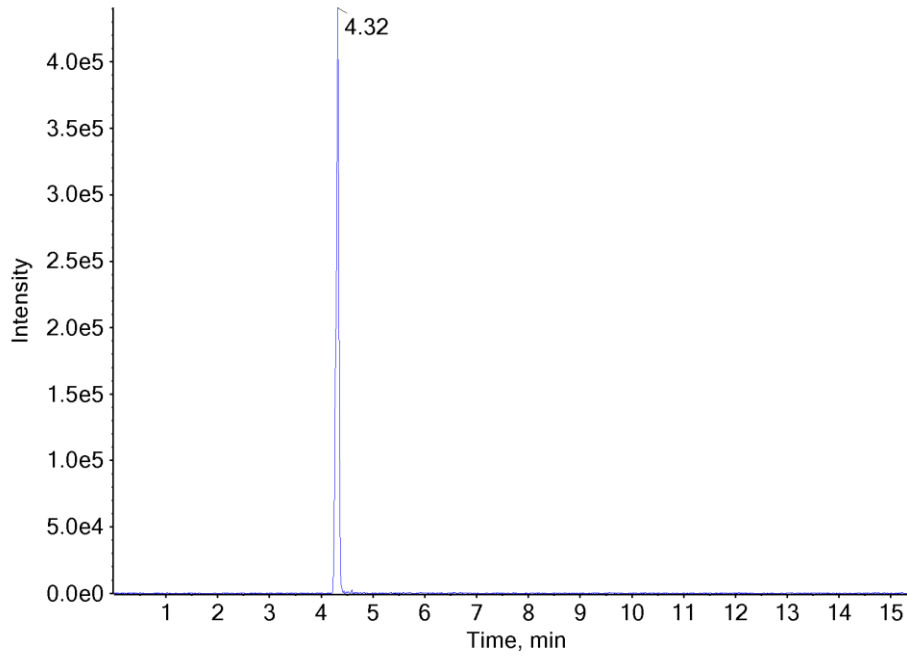
http://www.emcdda.europa.eu/system/files/publications/4724/TDAN17001ENN_PDFWEB.pdf

6. QUALITATIVE DATA

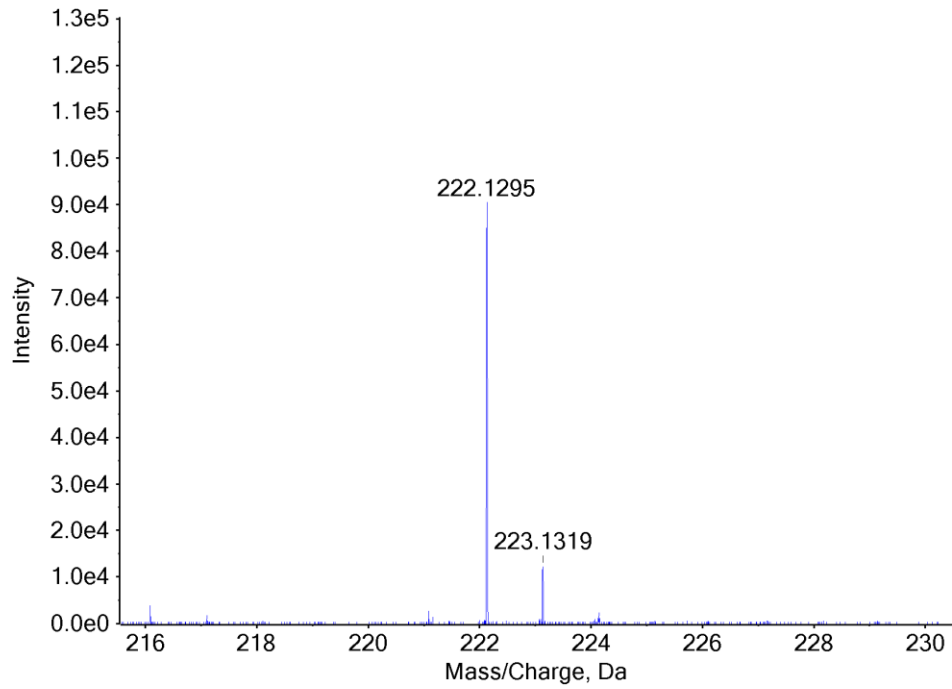
6.1 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	4.32 min
Standard Comparison:	Reference material for 2F-Deschloroketamine (Batch: 0504940-9) 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 2F-Deschloroketamine, based on retention time (4.21 min) and mass spectral data. (https://www.caymanchem.com/product/19786)

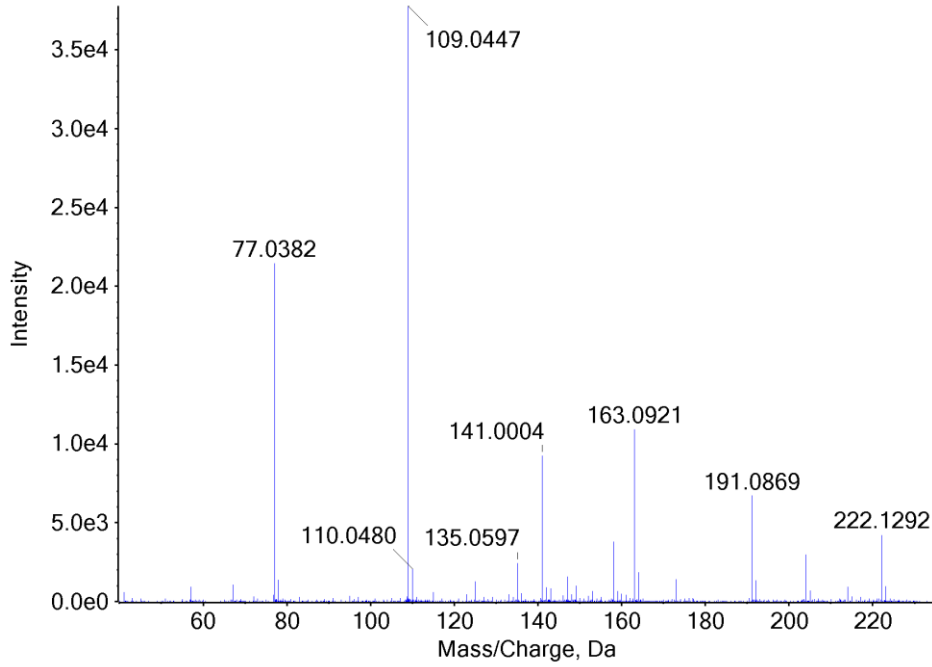
Extracted Ion Chromatogram: 2F-Deschloroketamine



TOF MS Spectrum: 2F-Deschloroketamine



MS/MS Spectrum: 2F-Deschloroketamine



7. FUNDING

This project was supported by Award Number 2017-R2-CX-0002, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication, program, or exhibition are those of the author(s) and do not necessarily reflect those of the Department of Justice.