

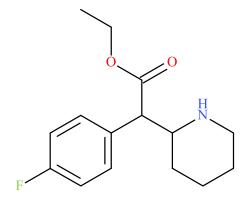
# 4F-Ethylphenidate

Sample Type: Seized Material

Latest Revision: May 7, 2020

Date Received: November 22, 2019

Date of Report: May 7, 2020



### 1. GENERAL INFORMATION

**IUPAC Name:** Ethyl 2-(4-fluorophenyl)-2-(2-piperidyl)acetate

**InChI String:** InChI=1S/C15H20FNO2/c1-2-19-15(18)14(13-5-3-4-10-17-

13)11-6-8-12(16)9-7-11/h6-9,13-14,17H,2-5,10H2,1H3

CFR: Not Scheduled (04/2020)

CAS# Not Available

**Synonyms:** 4-fluoro ethylphenidate, 4F-EPH

**Source:** Department of Homeland Security

**Appearance:** White Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS, and NMR), as no standard reference material was available at the time of testing. Delay between date of receipt and date of report may be due to the requirement of complex analytical testing for confirmation.

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#### 2. CHEMICAL AND PHYSICAL DATA

## 2.1 CHEMICAL DATA

Form	Chemical	Molecular	Molecular Ion	Exact Mass
	Formula	Weight	[M <sup>+</sup> ]	[M+H] <sup>+</sup>
Base	C <sub>15</sub> H <sub>20</sub> FNO <sub>2</sub>	265.3	265	266.1551

### 3. BRIEF DESCRIPTION

4F-Ethylphenidate is classified as a novel stimulant and analogue of methylphenidate (Ritalin). Novel stimulants have been reported to cause effects similar to amphetamine. Novel stimulants have caused adverse events, including deaths, as described in the literature. Structurally similar analogues of methylphenidate include ethylphenidate, 4-fluoromethylphenidate, and 3,4-dichloromethylphenidate. Methylphenidate is a Schedule II substance in the United States while 4F-ethylphenidate is not explicitly scheduled.

#### 4. ADDITIONAL RESOURCES

http://swgdrug.org/Monographs/4-Fluoroethylphenidate.pdf

https://www.policija.si/apps/nfl response web/0 Analytical Reports final/4-fluoroethylphenidate-ID-1602005\_report01.pdf

https://www.policija.si/apps/nfl\_response\_web/0\_Analytical\_Reports\_final/4F-EPH-ID-1563-16-report200616.pdf

## 5. QUALITATIVE DATA

#### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/Base extraction

**Instrument:** Agilent 5975 Series GC/MSD System

Column: Zebron<sup>TM</sup> Inferno<sup>TM</sup> ZB-35HT (15 m x 250  $\mu$ m x 0.25  $\mu$ m)

Carrier Gas: Helium (Flow: 1 mL/min)

**Temperatures:** Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:** Injection Type: Splitless

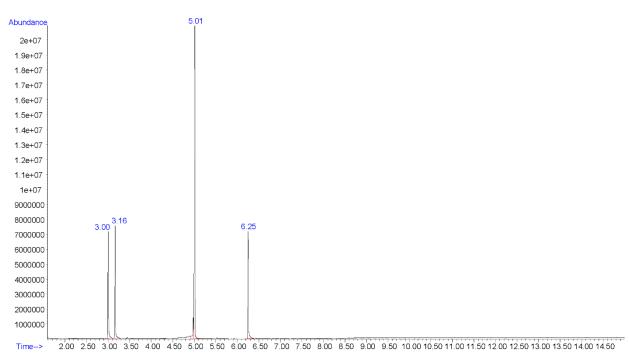
Injection Volume: 1 µL

**MS Parameters:** Mass Scan Range: 40-550 m/z

Threshold: 250

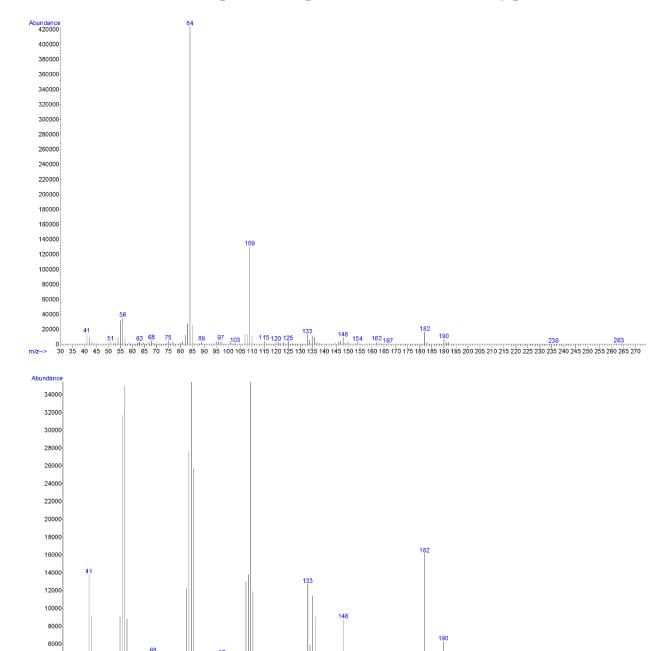
**Retention Time:** 5.01 min

## **Chromatogram: 4F-Ethylphenidate**



Additional peaks present in chromatogram: not a controlled substance (3.00 min), internal standard (3.16 min), and internal standard (6.25 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-Ethylphenidate



4000 2000

# **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:** 1:100 dilution of acid/base extract in mobile phase

**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

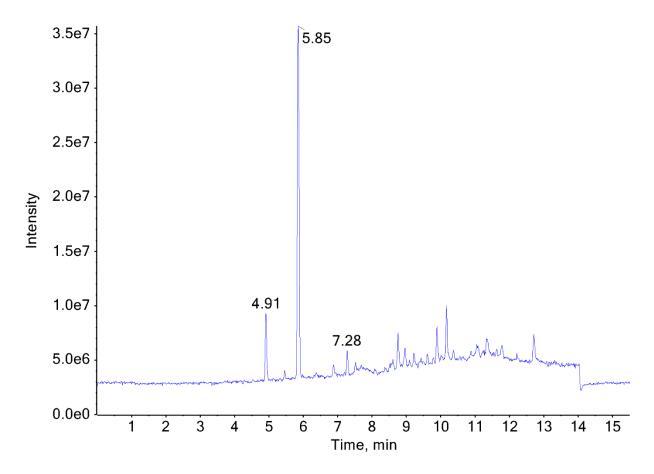
Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

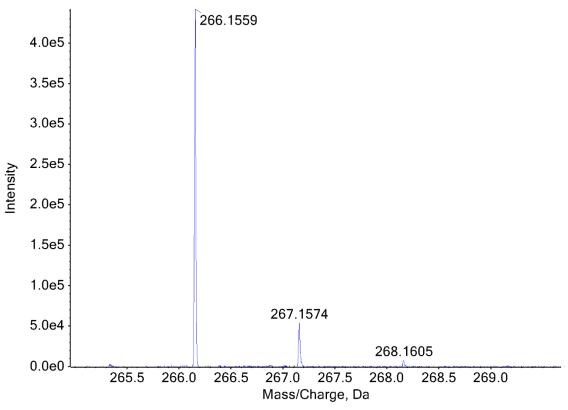
**Retention Time:** 5.85 min

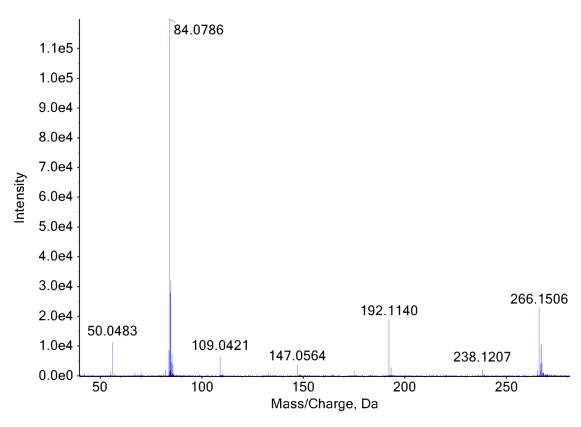
# **Chromatogram: 4F-Ethylphenidate**



Additional peaks present in chromatogram: internal standards (4.91 min and 7.28 min)







# **5.3 NUCLEAR MAGNETIC RESONANCE (NMR)**

**Testing Performed At:** IteraMed<sup>TM</sup> (Doylestown, PA)

**Sample Preparation:** Powder dissolved in CDCl<sub>3</sub>

**Instrument:** 600 MHz Bruker AVANCE<sup>TM</sup> III Spectrometer

**Parameters:** Pulse Sequence: Proton

Solvent: CDCl<sub>3</sub>

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for

<sup>1</sup>H; 36231.88 Hz = 240.0768 ppm = 0.552855 Hz/pt for <sup>13</sup>C; 5000.00 Hz = 8.3315 ppm = 2.4414 Hz/pt for COSY; 5000.00 Hz = 8.3315 ppm = 2.4414 Hz/pt for HSQC; 5000.00 Hz = 8.3315

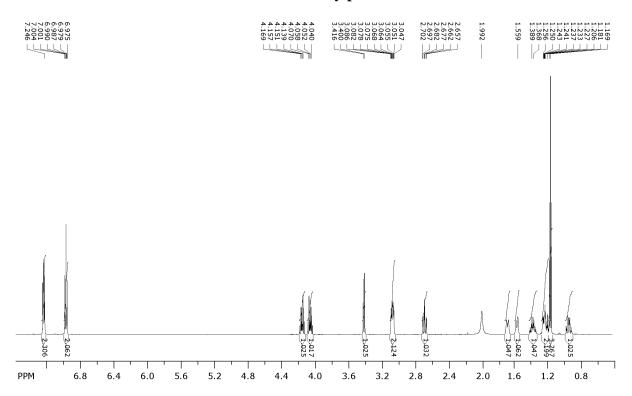
ppm = 1.6276 Hz/pt for HSQC

Number of Scans: 8 for <sup>1</sup>H; 1024 for <sup>13</sup>C; 2 for COSY; 2 for

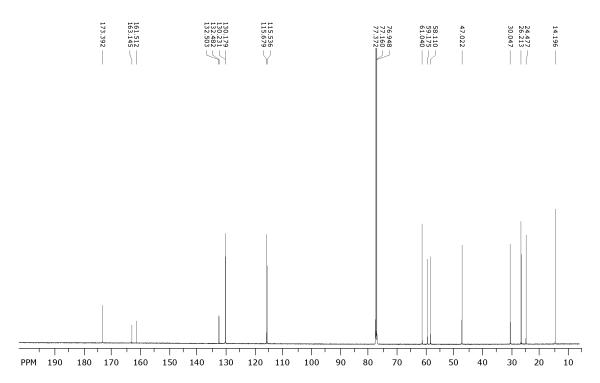
HSQC; 6 for HMBC

Delay Between Pulses: 1.000 second for <sup>1</sup>H, 2.000 seconds for <sup>13</sup>C

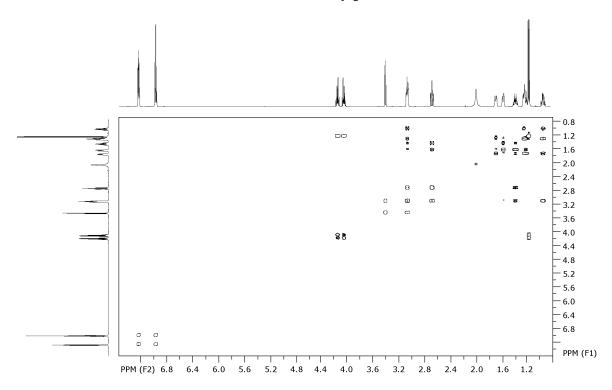
## <sup>1</sup>H NMR: 4F-Ethylphenidate



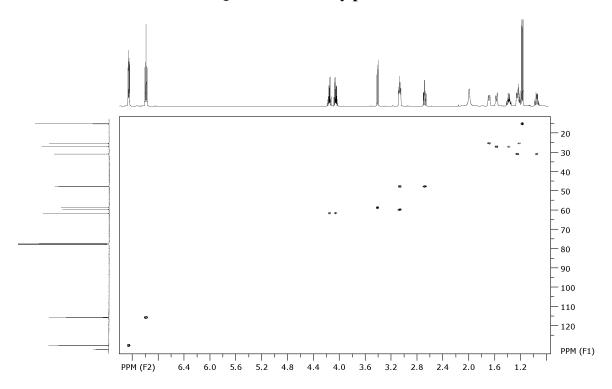
# <sup>13</sup>C NMR: 4F-Ethylphenidate



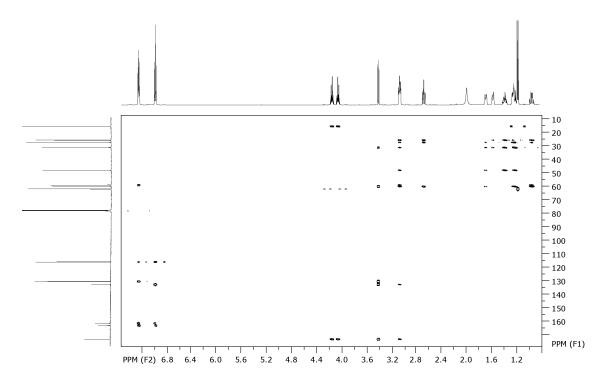
# **COSY NMR: 4F-Ethylphenidate**



**HSQC NMR: 4F-Ethylphenidate** 



**HMBC NMR: 4F-Ethylphenidate** 



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