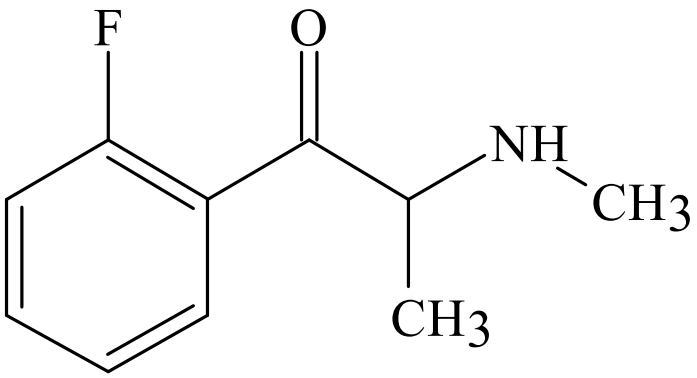
2-Fluoromethcathinone

Latest Revision: April 5, 2013



1. GENERAL INFORMATION

IUPAC Name: 1-(2-fluorophenyl)-2-(methylamino)propan-1-one

CFR: Not Scheduled (3/2013)

CAS#: To Be Determined

Synonyms: 2-FMC

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: 246.2, 289.3

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{10}H_{12}FNO$	181	Not Determined
HCl	$C_{10}H_{12}FNO \cdot HCl$	217	129.1

3. ADDITIONAL RESOURCES

Kolodziejczyk W, Jodkowski J, Holmes TM, Hill GA. Conformational analysis of flephedrone using quantum mechanical models.*J Mol Model*. 2013; 19:14511458.

Tsujikawa K, Mikuma T, Kuwayama K,*et al*. Identification and differentiation of methcathinone analogs by gas chromatography-mass spectrometry. *Drug Test. Analysis*. 2012; doi 10.1002/dta.1437.

Westphal F, Junge T. Ring positional differentiation of isomeric N-alkylated fluorocathinones by gas chromatography/tandem mass spectrometry. *Forensic Sci Intl. 2012;* 223: 97-105.

Tsujikawa K, Mikuma T, Kuwayama K, et al. Degradation pathways of 4-methylmethcathinone in alkaline solution and stability of methcathinone analogs in various pH solutions.*Forensic Sci Intl*. 2012; 220: 103-110.

Zuba D. Identification of cathinones and other active components of legal highs by mass spectrometric methods. *Trends Anal. Chem*. 2012; 32: 15-30.

Westphal F, Rosner P Junge Th. Differentiation of regioisomeric ring-substituted fluoro phenethylamines with product ion spectrometry. *Forensic Sci Intl*. 2010; 194: 53-59.

Archer RP. Fluoromethcathinone, a new substance of abuse. *Forensic Sci. Intl.* 2009; 185(1): 10-20.

Noggle FT, DeRuiter J, Valaer A, Clark CR. GC-MS analysis of methcathinone and its major decomposition product. 1994; 27(4): 106-118.

4. QUALITATIVE DATA

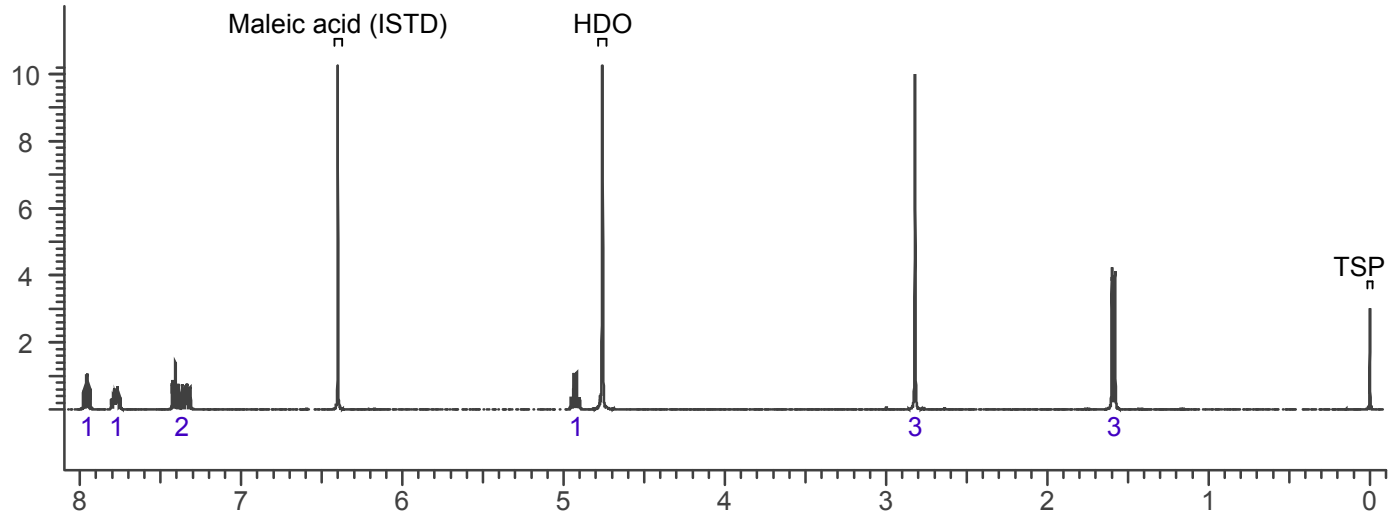
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

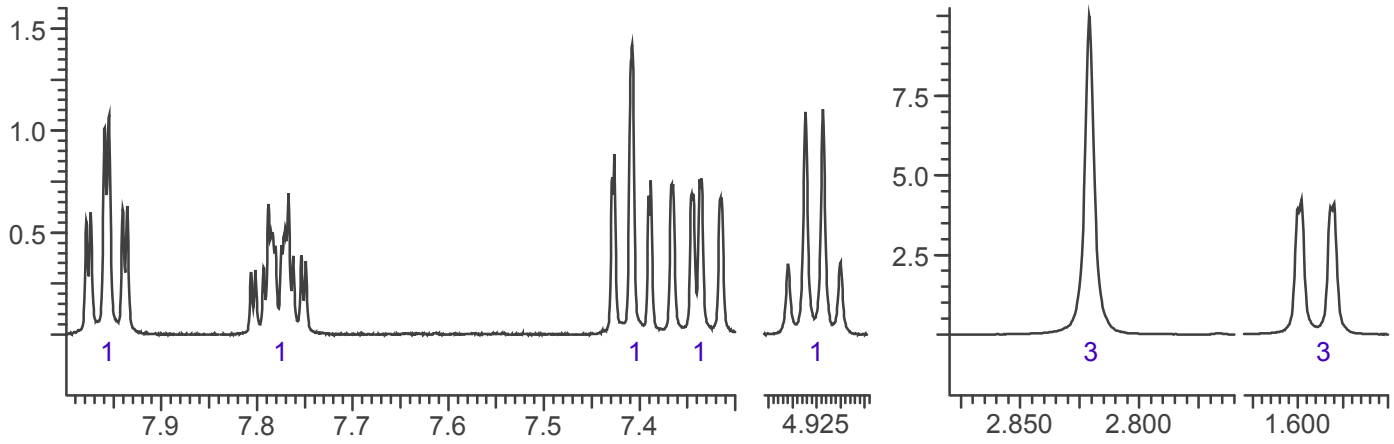
Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}H NMR: 2-Fluoromethcathinone HCl; lot TAD2FL1; D_2O, 400 MHz



^{1}H NMR: 2-Fluoromethcathinone HCl; lot TAD2FL1; D_2O, 400 MHz

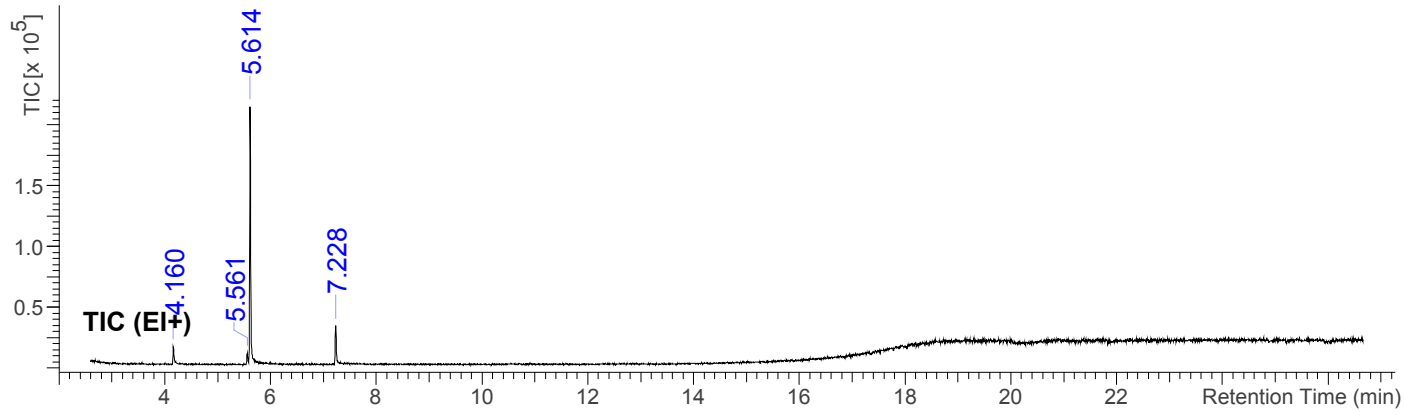


4.2 Gas Chromatography/Mass Spectrometry

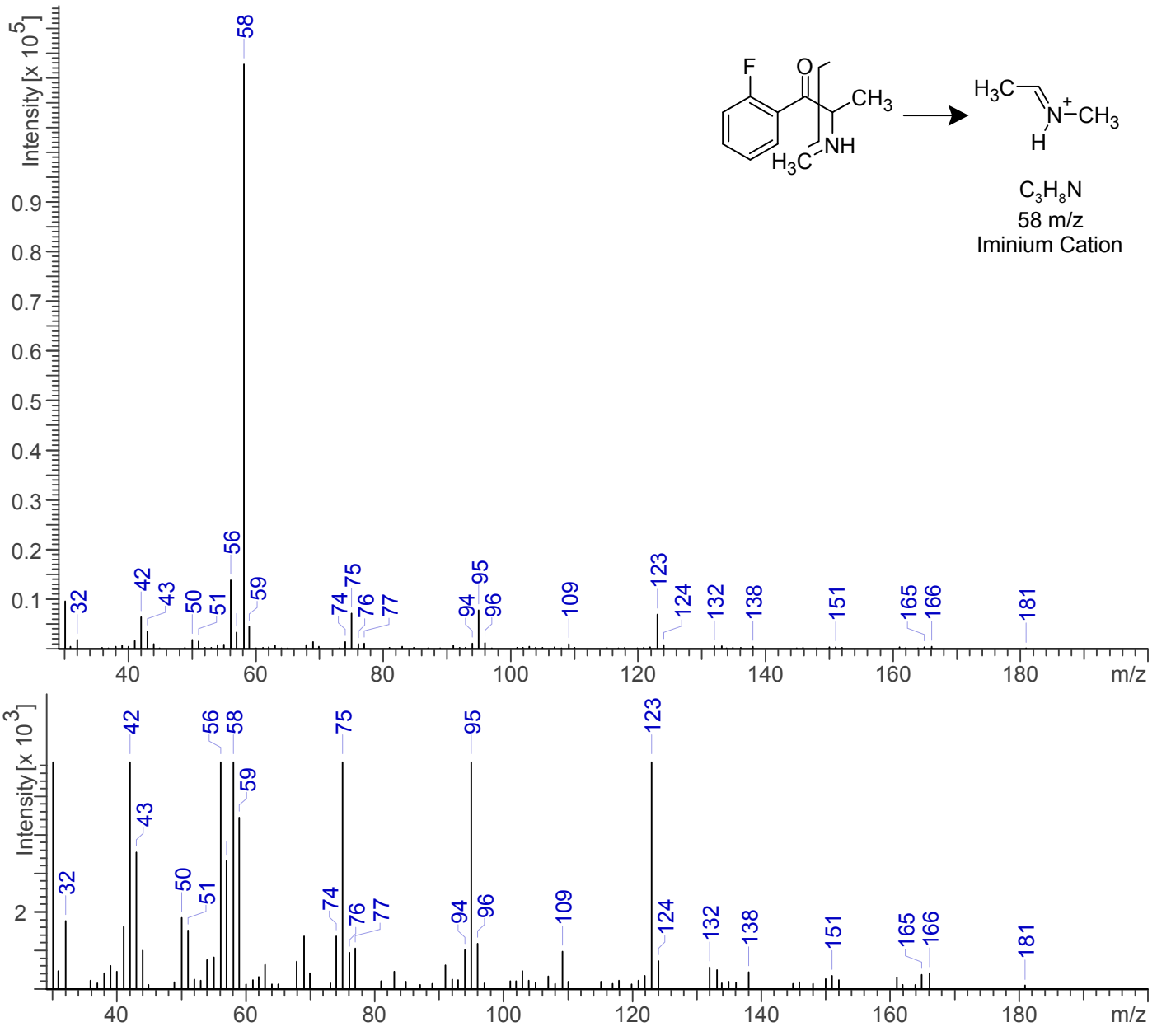
Sample Preparation: Dilute analyte ~1 mg/mL base extracted into chloroform.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12 °C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 20:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	5.614 min

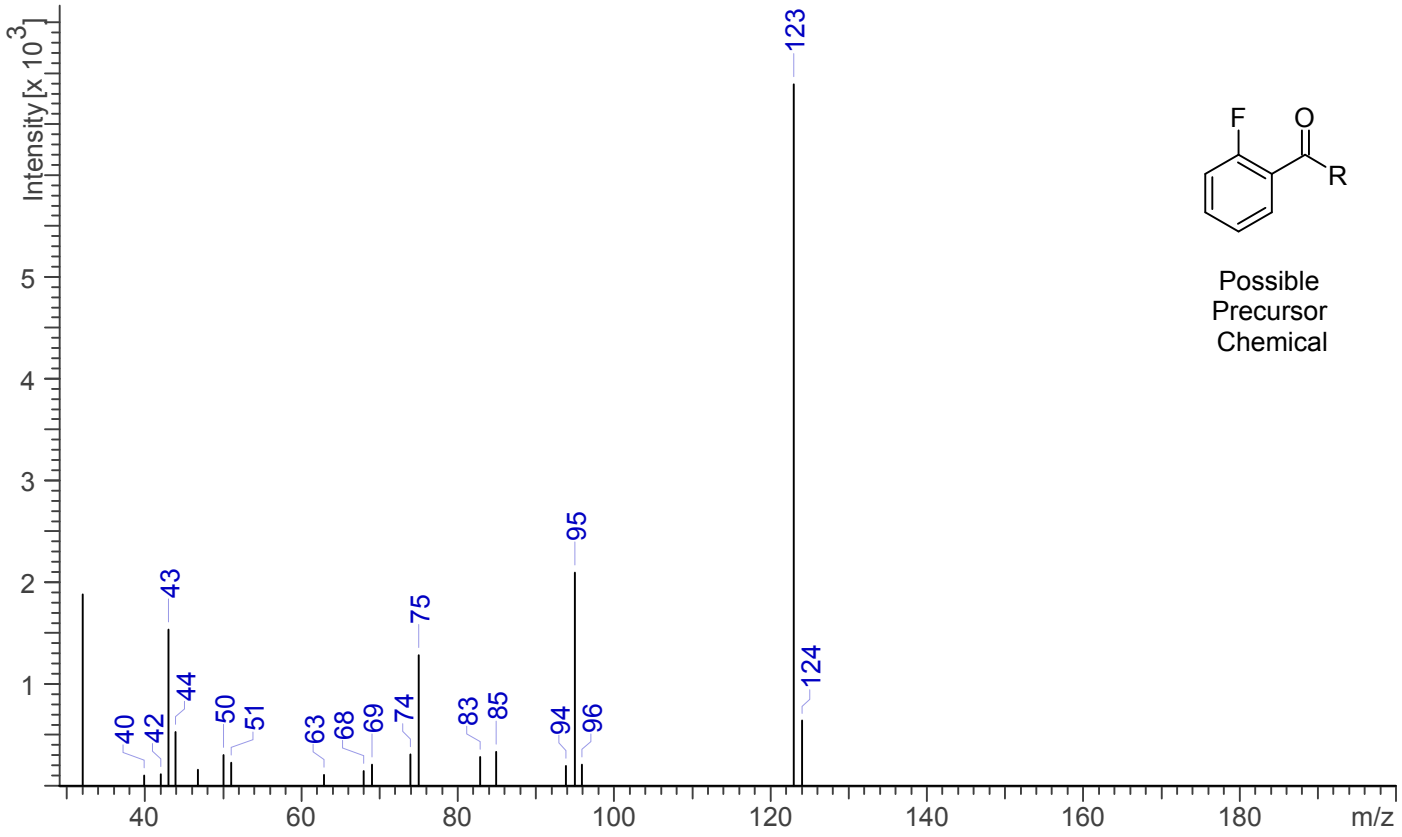
Total Ion Chromatogram: 2-fluoromethcathinone; lot TAD2FL1



EI Mass Spectrum: 2-fluoromethcathinone HCl; lot TAD2FL1; 5.614 min

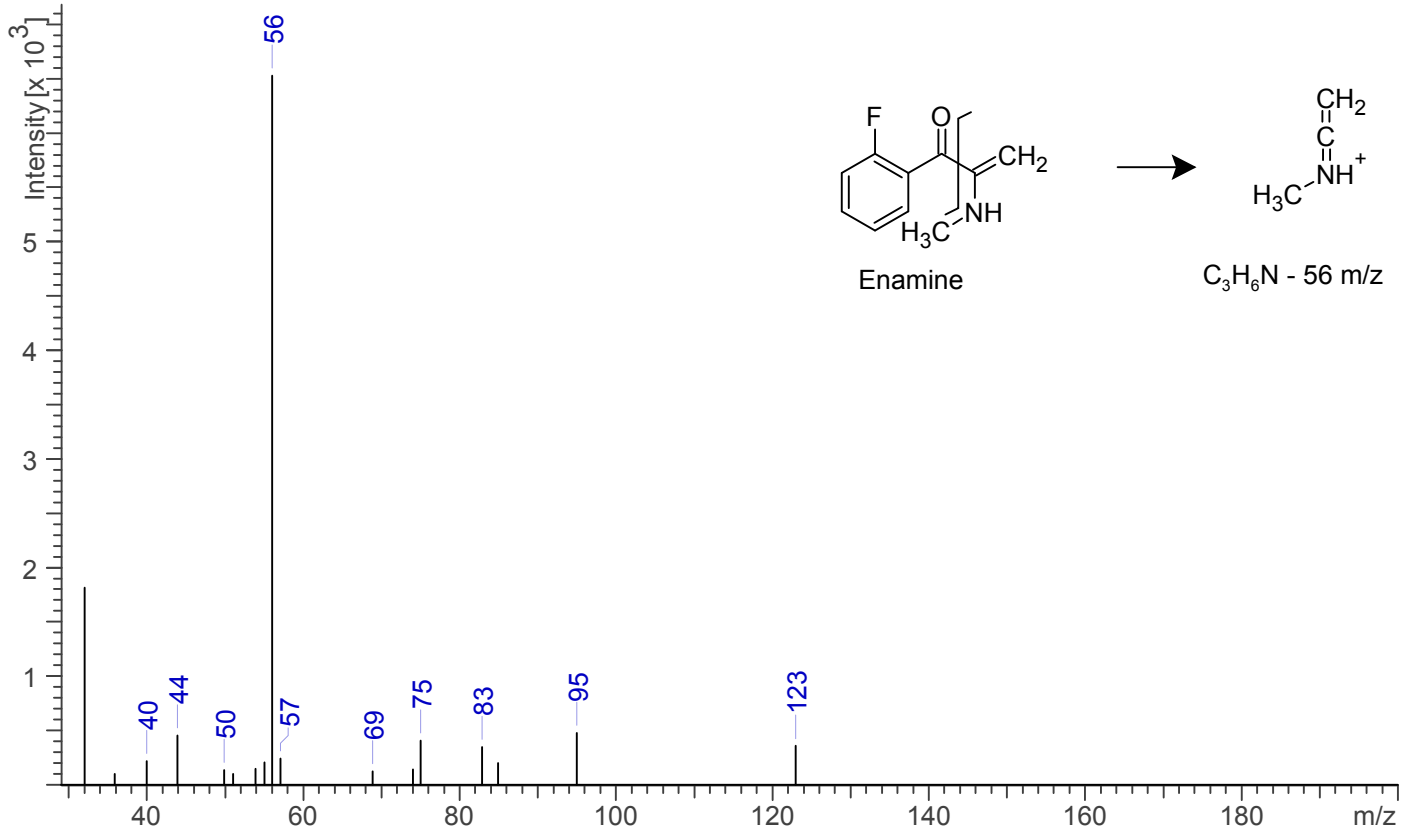


EI Mass Spectrum: 2-fluoromethcathinone HCl; lot TAD2FL1; 4.160 min



Possible Precursor Chemical

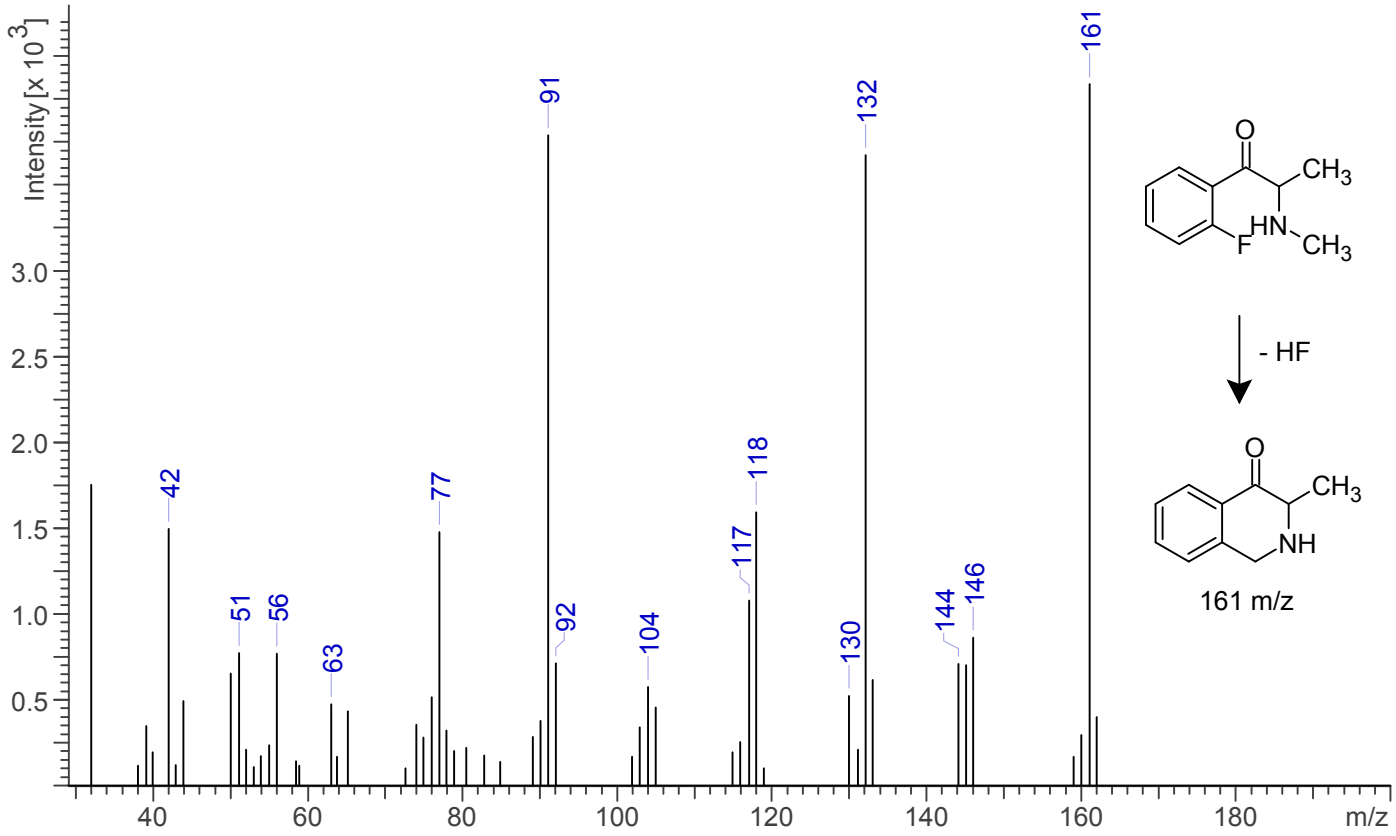
EI Mass Spectrum: 2-fluoromethcathinone HCl; lot TAD2FL1; 5.561 min



Enamine

C_3H_6N - 56 m/z

EI Mass Spectrum: 2-fluoromethcathinone HCl; lot TAD2FL1; 7.228 min



GC/MS Analytical Observation:

2-Fluoromethcathinone decomposes in the GC/MS. Upon comparison with other phenethylamines, the mass spectrum at 5.617 minutes, mainly resulting from α-cleavage, is the expected spectrum. A possible precursor chemical is indicated at 4.160 minutes which is possibly 2-fluorobenzaldehyde or 1-(2-fluorophenyl)propan-1-one. Cathinones can lose two hydrogens to produce an enamine that undergoes α-cleavage to yield a mass spectrum with a base peak of 56 m/z for methcathinones (see the mass spectrum at 5.561 minutes).[1] The enamine compound can also be due to a reaction by-product. Ortho fluorophenethylamines undergo a ring closure with the loss of HF.[2] 2-Fluoromethcathinone forms an energetically favorable six membered ring, with the resulting mass spectrum at 7.228 minutes.[3]

[1]Noggle FT, DeRuiter J, Valaer A, Clark CR. GC-MS analysis of methcathinone and its major decomposition product. 1994; 27(4): 106-118.
[2]Westphal F, Rosner P Junge Th. Differentiation of regioisomeric ring-substituted fluoro phenethylamines with product ion spectrometry. *Forensic Sci Intl*. 2010; 194: 53-59.
[3]Tsujikawa K, Mikuma T, Kuwayama K,*et al*. Identification and differentiation of methcathinone analogs by gas chromatography-mass spectrometry. *Drug Test. Analysis*. 2012; doi 10.1002/dta.1437.

4.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 bounce): 2-fluoromethcathinone HCl; lot TAD2FL1