

1. GENERAL INFORMATION

IUPAC Name:	1-(3-fluorophenyl)-2-methylaminopropan-1-one
CFR:	Not Scheduled (3/2013)
CAS #:	1049677-77-1
Synonyms:	3-FMC
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's Index:	Pending
UV_{max} (nm):	247.5, 291.1

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₀ H ₁₂ FNO	181	Not Determined
HCl	C ₁₀ H ₁₂ FNO · HCl	217	169.3

3. ADDITIONAL RESOURCES

Marinetti LJ, Antonides HM. Analysis of synthetic cathinones commonly found in bath salts in human performance and postmortem toxicology: method development, drug distribution and interpretation of results. *J Analytical Toxicology*. 2013; 37: 135-146.

Kolodziejczyk W, Jodkowski J, Holmes TM, Hill GA. Conformational analysis of flephedrone using quantum mechanical models. *J Mol Model*. 2013; 19:1451–1458.

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.

Davis S, Rands-Trevor K, Boyd S, Edirisinghe M. The characterisation of two halogenated cathinone analogues: 3,5-Difluoromethcathinone and 3,5-dichloromethcathinone *Forensic Sci Intl*. 2012; 217: 139-145.

Pawlik E, Plässer G, Mahler H, Daldrup T. Erratum to: Studies on the phase I metabolism of the new designer drug 3-fluoromethcathinone using rabbit liver slices. *Int J Legal Med*. 2012; 126: 241-242.

Pawlik E, Plässer G, Mahler H, Daldrup T. Studies on the phase I metabolism of the new designer drug 3-fluoromethcathinone using rabbit liver slices. *Int J Legal Med*. 2012; 126: 231-240.

Meyer MR, Vollmar C, Schwaninger AE, Wolf E, Maurer HH. New cathinone-derived designer drugs 3-bromomethcathinone and 3-fluoromethcathinone: studies on their metabolism in rat urine and human liver microsomes using GC-MS and LC-high-resolution MS and their detectability in urine. *J Mass Spectrom*. 2012; 47: 253-262.

Marusich JA, Grant KR, Blough BE, Wiley JL. Effects of synthetic cathinones contained in “bath salts” on motor behavior and a functional observational battery in mice. *Neuro Toxicology*. 2012; 33: 1305-1313.

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

Sørensen LK. Determination of cathinones and related ephedrine in forensic whole-blood samples by liquid-chromatography–electrospray tandem mass spectrometry. *Journal of Chromatography B*. 2011; 879: 727–736.

Westphal F, Junge T, , Girreser U, Jacobsen-Bauer A, Rösner P. “Bathsalts” for snorting – fluoromethcathinone – now on the german illegal drug market. *TIAFT BULLETIN*. 2010; 40(2): 28-33.

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

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR ($CDCl_3$)

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

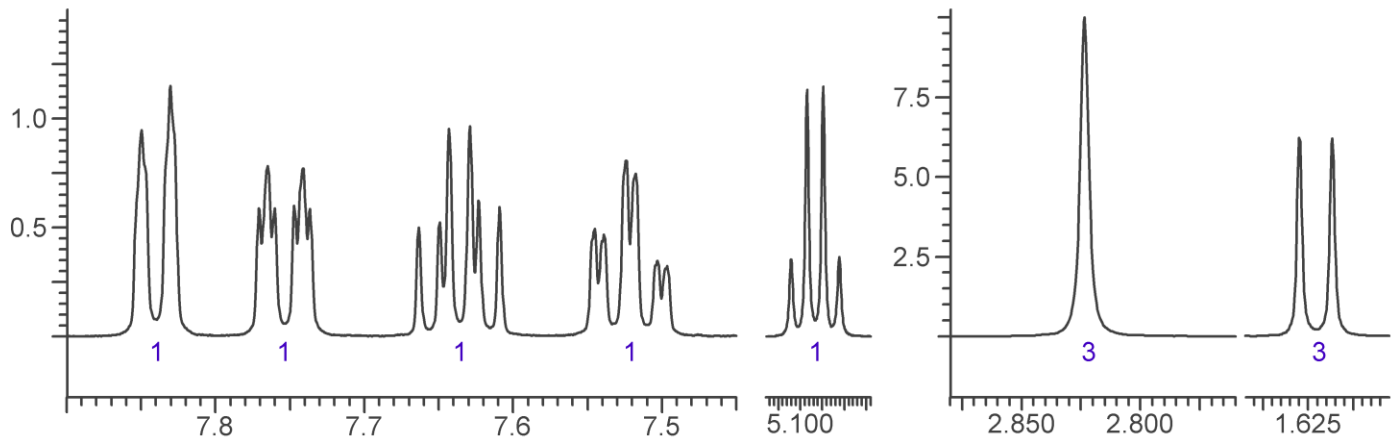
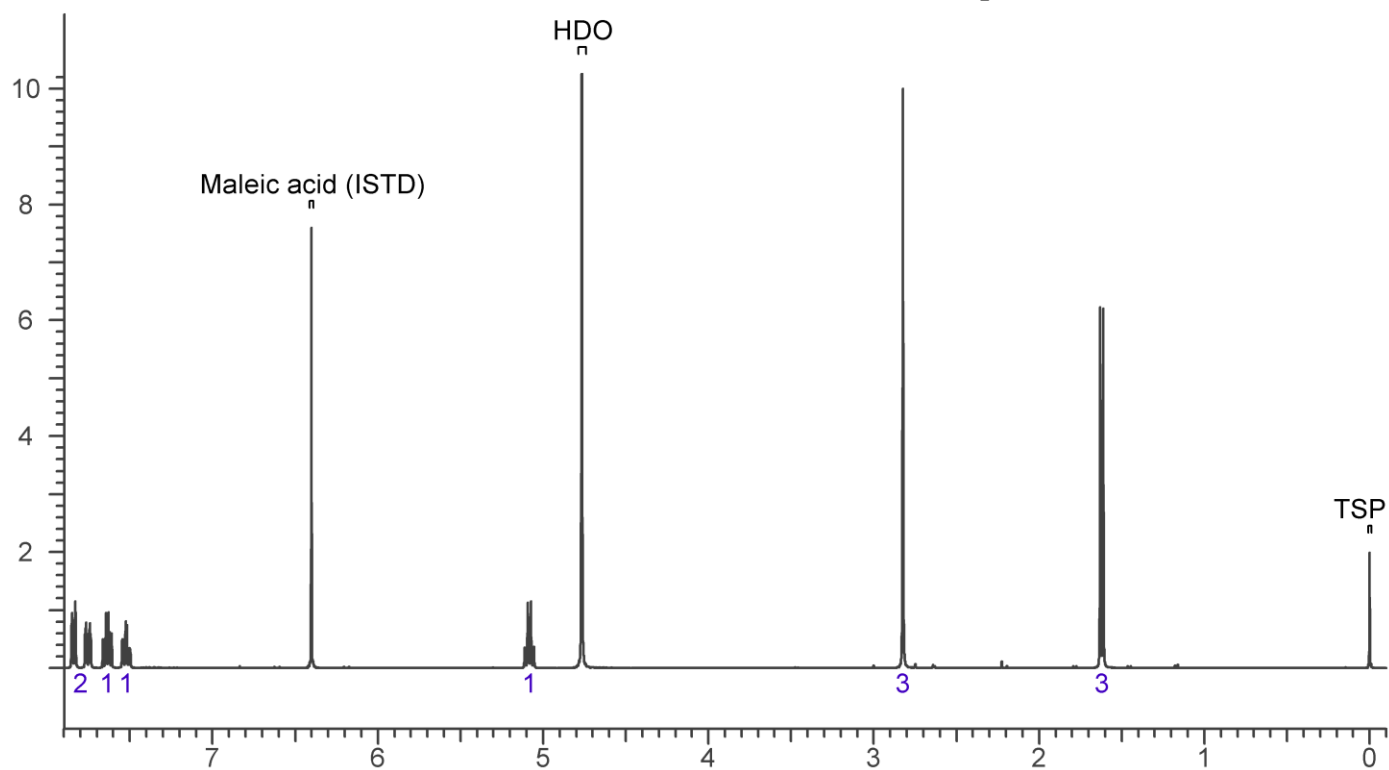
Parameters:

Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

1H NMR: 3-Fluoromethcathinone HCl; lot TAD3FLU1; 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 μ m

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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

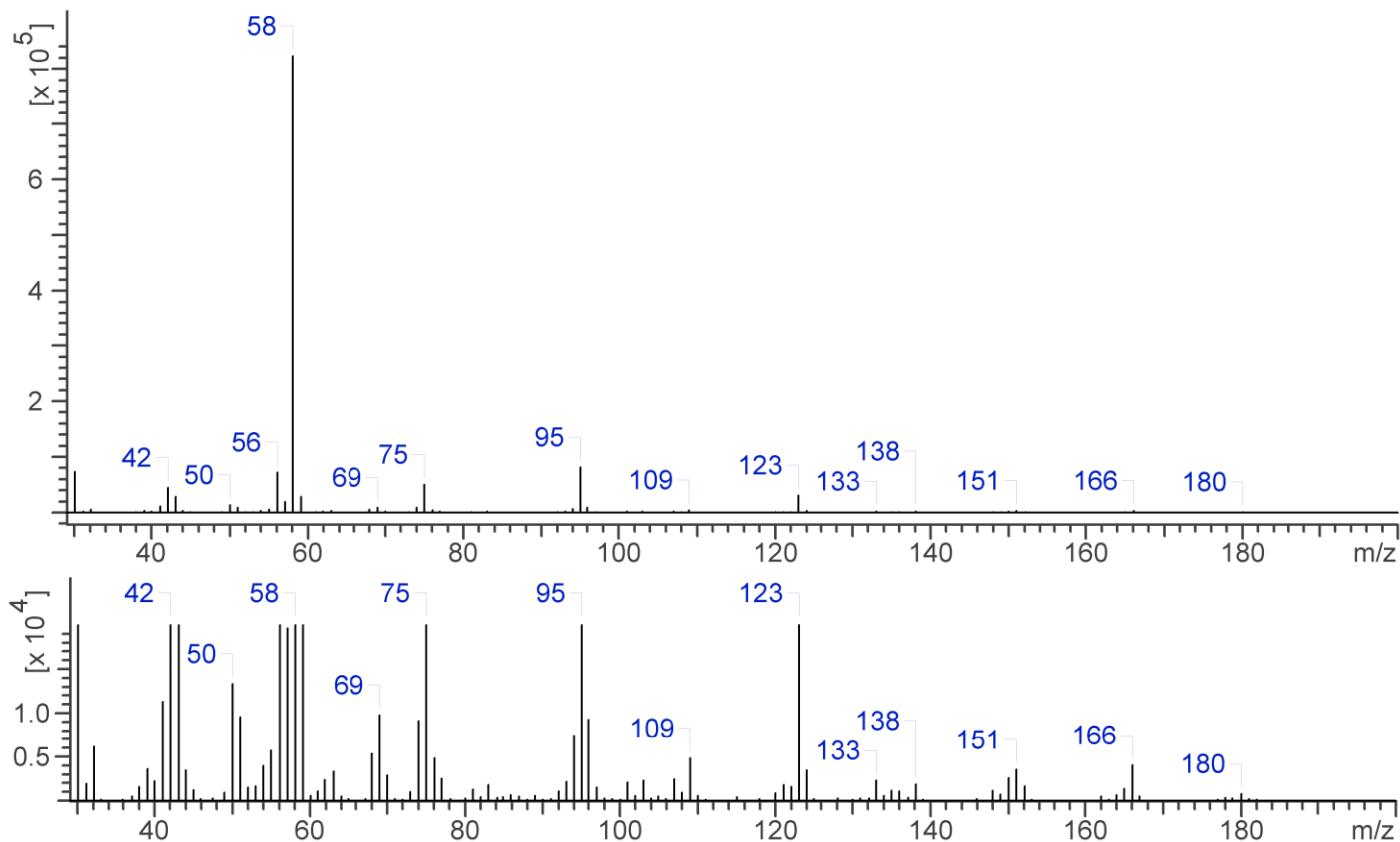
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 5.692 min

EI Mass Spectrum: 3-Fluoromethcathinone HCl; lot TAD3FLU1



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: 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): 3-Fluoromethcathinone HCl; lot TAD3FLU1

