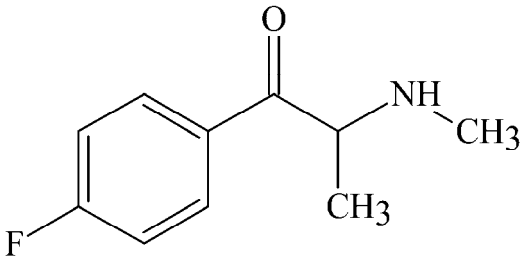
4-Fluoromethcathinone

Latest Revision: March 25, 2013



1. GENERAL INFORMATION

IUPAC Name: 1-(4-fluorophenyl)-2-methylaminopropan-1-one

CFR: Not Scheduled (3/2013)

CAS #: 7589-35-7

Synonyms: 4-FMC, flephedrone

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max} (nm): 253.6

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	$C_{10}H_{12}FNO \cdot HCl$	217	230.0

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.

Thornton SL, Gerona RR, Tomaszewski CA. Psychosis from a bath salt product containing flephedrone and MDPV with serum, urine, and product quantification. 2012; 8: 310-313.

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.

Brandt SD, Freeman S, Sumnall HR, Measham F, Cole J. Analysis of NRG ‘legal highs’ in the UK: Identification and formation of novel cathinones. *Drug Test. Analysis.* 2011, *3*, 569–575.

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

Brandt SD, Sumnall HR, Measham F, Cole J. Analyses of second-generation ‘legal highs’ in the UK: Initial findings. *Drug Test. Analysis*. 2010; 2: 377-382.

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

Forendex

Wikipedia

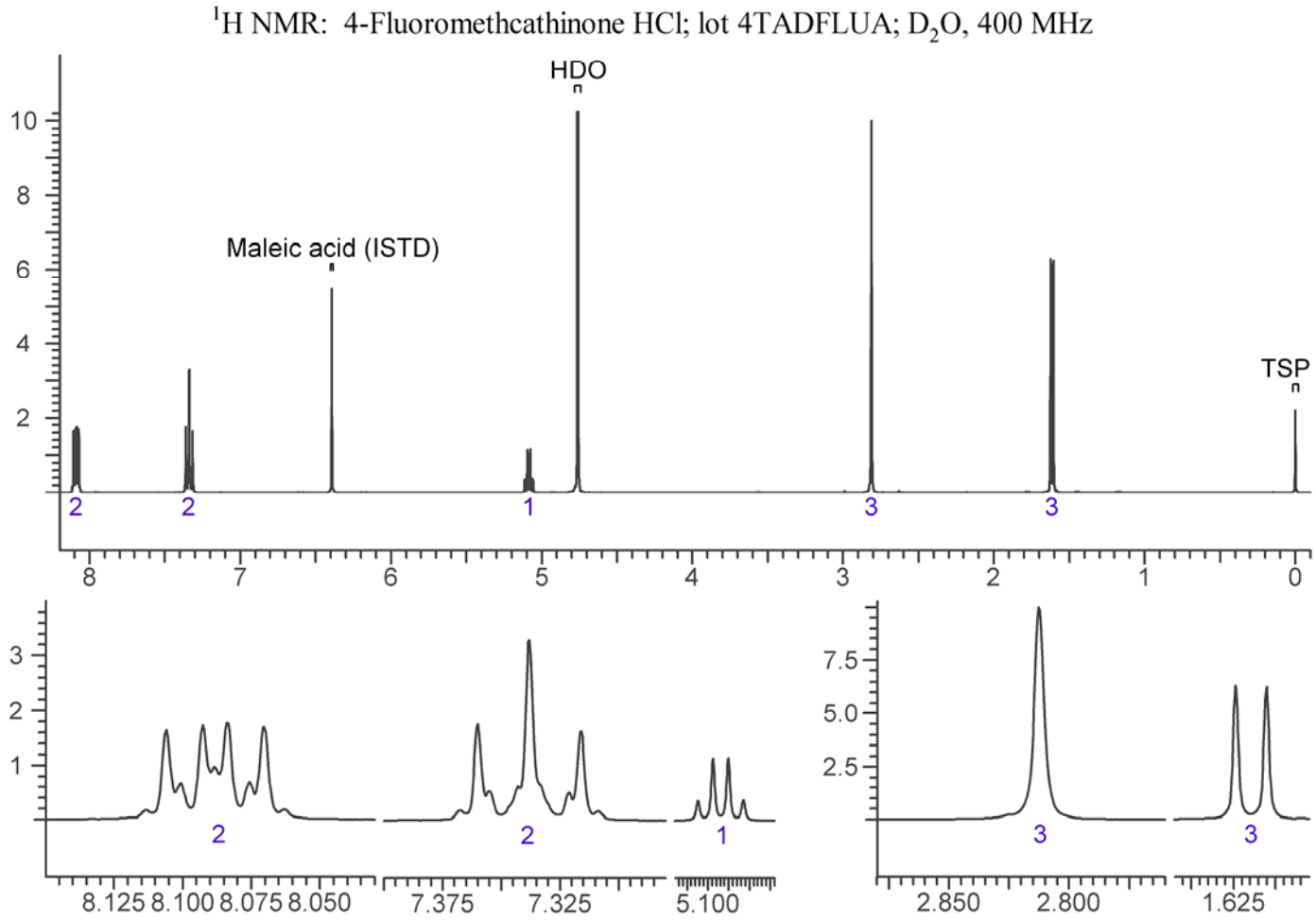
4. QUALITATIVE DATA

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

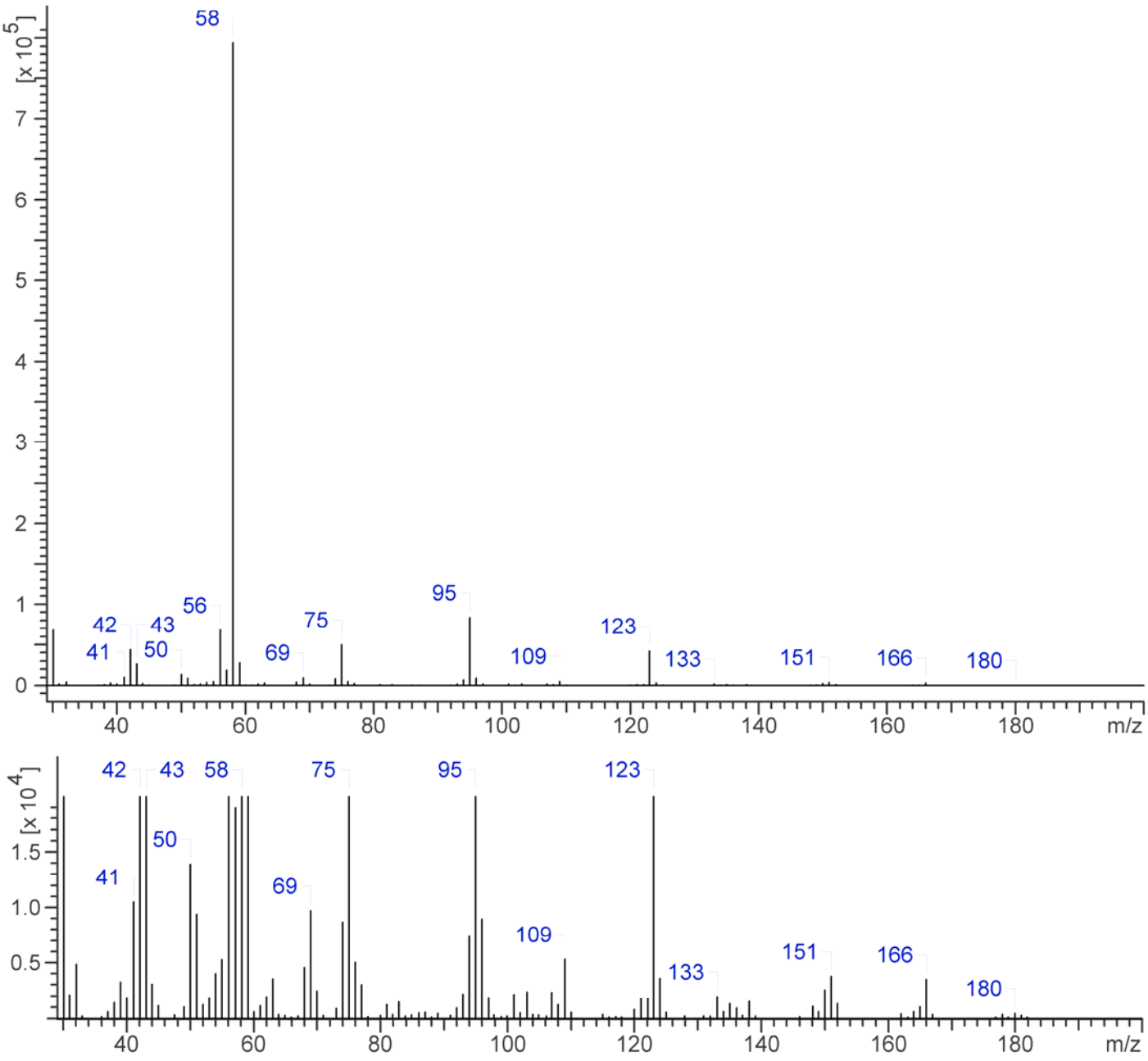


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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:	5.739 min

EI Mass Spectrum: 4-fluoromethcathinone HCl; lot 4TADFLUA



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): 4-fluoromethcathinone HCl; lot 4TADFLUA