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NACIONALNI FORENZIČNI LABORATORIJ

Vodovodna 95 1000 Ljubljana SLOVENIJA

T: +386 (0)1 428 44 93 E: <u>nfl@policija.si</u> www.policija.si

ANALYTICAL REPORT

2-Fluoromethcathinone (C10H12FNO)

1-(2-fluorophenyl)-2-(methylamino)propan-1-one

Remark – other active cpd. detected: none

Sample ID:	1470-16
Sample description:	liquid - clear
Sample type:	RM-reference material
Comments ¹ :	LGC Lot#11474; compound was partially disproportionatedI-SEE - purchasing
Date of entry:	2/19/2016

Substance identified- structure ² (base form)				
Systematic name:	1-(2-fluorophenyl)-2-(methylamino)propan-1-one			
Other names:	2-FMC			
Formula (per base form)	C10H12FNO			
M _w (g/mol)	181.21			
Salt form:	HCI			
StdInChIKey	DCMOUMKIDLRIBO-UHFFFAOYSA-N			
Compound Class	Cathinones			
Other active cpd. detected	none			
Add.info (purity)	1mg/ml in MeOH			
	(in GC compound partially disproportionate; see in FSI 194 (2010, p 53-58) and figures			
	below, pure by HPLC-TOF			

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² Created by OPSIN free tool: <u>http://opsin.ch.cam.ac.uk/</u> **DOI:** 10.1021/ci100384d





Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (El ionization)	+	NFL GC-RT (min): 2.81 BP(1): 58; BP(2): 56,BP(3) :95,
HPLC-TOF	+	(results not enclosed)

GC-MS (Agilent):

GC-method is RT locked to tetracosane (RT=9.53 min).

Injection volume 1 ml and split mode (1:50).

Injector temperature: 280 °C. Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235° C, source and quadropole temperatures 280° C and 180° C. respectively. Scan range m/z scan range: from 50 (30 until 6 min) to 550 (300) amu.

HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min: sheath gas flow rate 8 l/min: nebulizer 25 psig: Vcap. 4000 V: nozzle 2000 V: skimmer 65 V: fragmentor 175 V and Octopole RF 750 V.

FIGURES OF SPECTRA



Chromatogram: 2-fluoromethcathinone at 2.81 min and 1-(2-fluorophenyl)propan-1-one at 3.66 min



MS spectrum of 2-FMC at 2.81 min



MS spectrum of 1-(2-fluorophenyl)propan-1-one at 3.66 min