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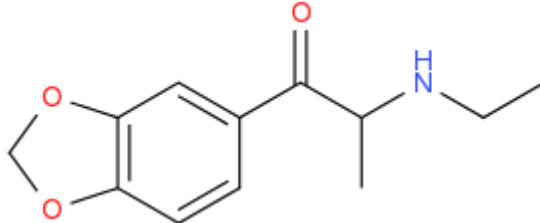
ANALYTICAL REPORT

Ethylone (C₁₂H₁₅N₃O₃)

(RS)-1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one

Remark – other active cpd. detected: **none**

Sample ID:	1107-14A
Sample description:	powder - white
Sample type:	RM-reference material
Comments:	LGC Lot#24827;
Date of entry:	9/22/2014

Substance identified-structure ¹ (base form)	
Systematic name:	(RS)-1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one
Other names:	
Formula (per base form)	C ₁₂ H ₁₅ N ₃ O ₃
M _w (g/mol)	221,25
Salt form:	HCl
StdInChIKey	MJEMIOXXNCZZFK-UHFFFAOYSA-N
Compound Class	Cathinones
Other active cpd. detected	none
Add.info (purity..)	98,40%

¹ Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d



Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 5,53 BP(1): 72; BP(2): 44,BP(3) :149,
FTIR-ATR	+	direct measurement

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 thickness 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, then 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 (40) to 550 amu.

FTIR-ATR (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm⁻¹

GC-method:

Injection volume 1 ml and split mode (1:5) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 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, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

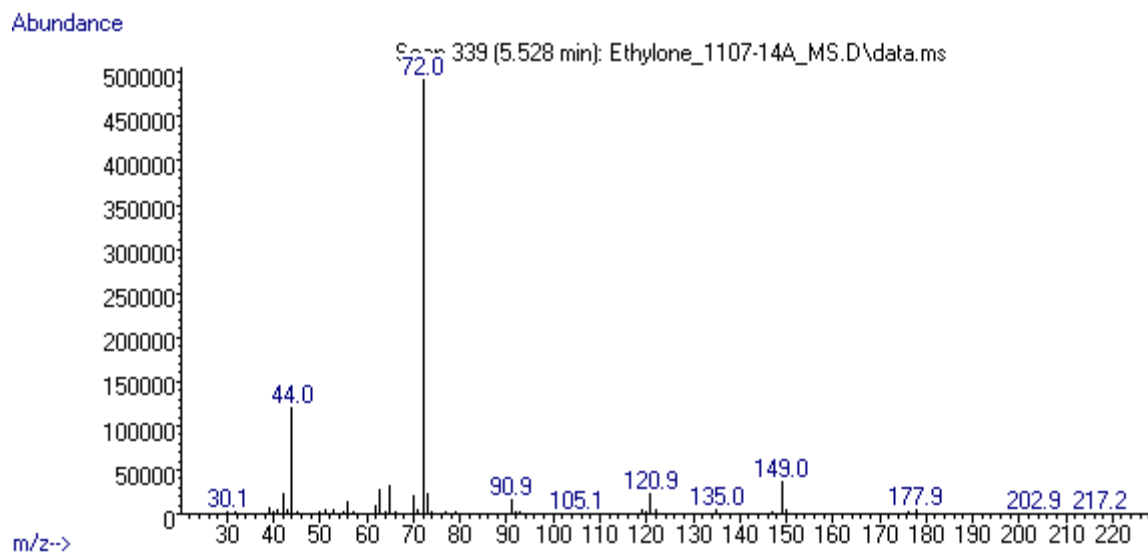
Split MS : IR : (1:9)

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 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 700, resolution 4cm⁻¹

FIGURES OF SPECTRA

MS (EI)



FTIR-ATR

