

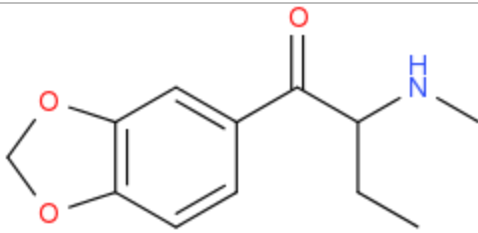
ANALYTICAL REPORT

Butylone (C₁₂H₁₅N₃O₃)

1-(1,3-benzodioxol-5-yl)-2-(methylamino)butan-1-one

Remark – other NPS detected: **none**

Sample ID:	1079-13A
Sample description:	powder - white
Sample type:	RM-reference material
Comments:	NMI Australia Lot#09-D-22
Date of entry:	11/28/2013

Substance identified-structure ⁱ (base form)	
Systematic name	1-(1,3-benzodioxol-5-yl)-2-(methylamino)butan-1-one
Other names	
Formula (per base form)	C ₁₂ H ₁₅ N ₃ O ₃
M _w (g/mol)	257,7 (salt form); 221,26 (base form)
Salt form	HCl
Smiles	<chem>O1COC2=C1C=CC(=C2)C(C(CC)NC)=O</chem>
Compound Class	Cathinones
Other NPS detected	none
Add.info (purity..)	99,30%

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Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 5,64 BP(1): 72; BP(2): 149,BP(3) :57,
FTIR-ATR	+	

GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50) for GC-MS instruments and 1:5 for GC-MS-FTIR(condensed phase). Injector temperature: 280 °C. 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. m/z scan range: from 50 (40) to 550 amu.

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

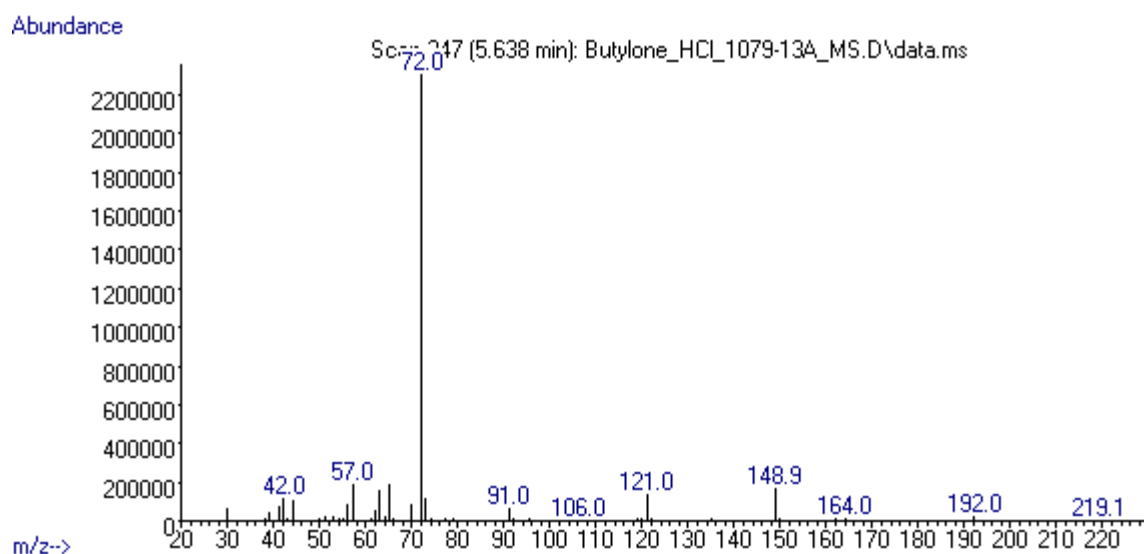


Figure 1: GC-MS spectrum

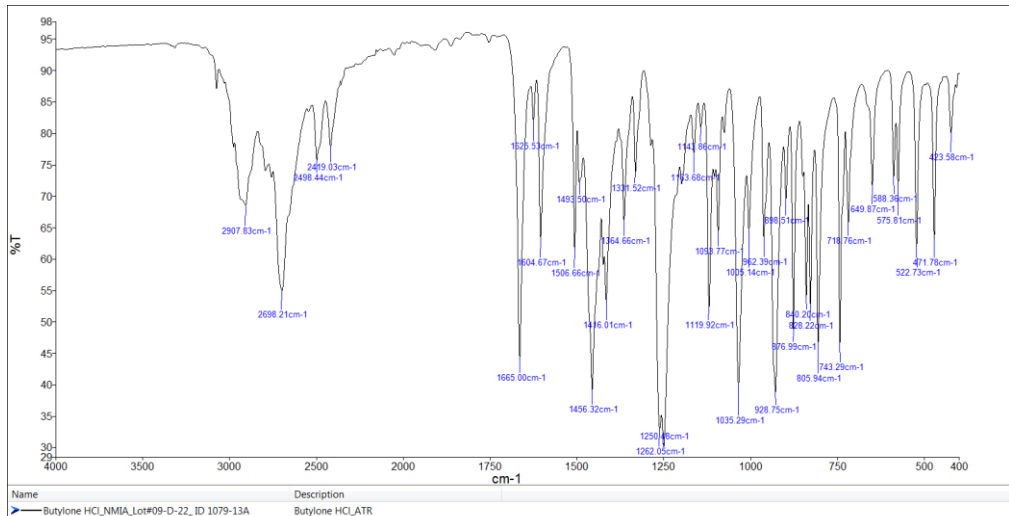


Figure 2: FTIR ATR

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