

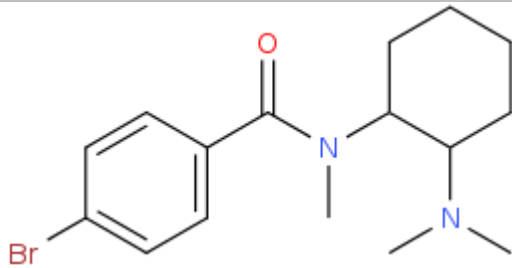
ANALYTICAL REPORT

N-methyl U-47931E (C₁₆H₂₃BrN₂O)

4-bromo-N-[2-(dimethylamino)cyclohexyl]-N-methylbenzamide

Remark – other active cpd. detected: none

Sample ID:	1917-18
Sample description:	powder - white
Sample type:	RM-reference material
Comments:	CAY Lot#0521838-3,
Date of entry (DD/MM/YYYY):	09/04/2018

Substance identified-structure ¹ (base form)	
Systematic name:	4-bromo-N-[2-(dimethylamino)cyclohexyl]-N-methylbenzamide
Other names:	trans-4-bromo-N-[2-(dimethylamino)cyclohexyl]-N-methyl-benzamide
Formula (per base form)	C ₁₆ H ₂₃ BrN ₂ O
M _w (g/mol)	339,28
Salt form:	base
StdInChIKey (per base form)	XQCGUPNNNXRBDG-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	100 %

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): 9,17 BP(1): 84; BP(2): 125,BP(3) :71,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form
HPLC-TOF	+	exact monoisotopic mass: 338,0994 Δ ppm (difference from calculated): 0,4

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

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

3. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1 : 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

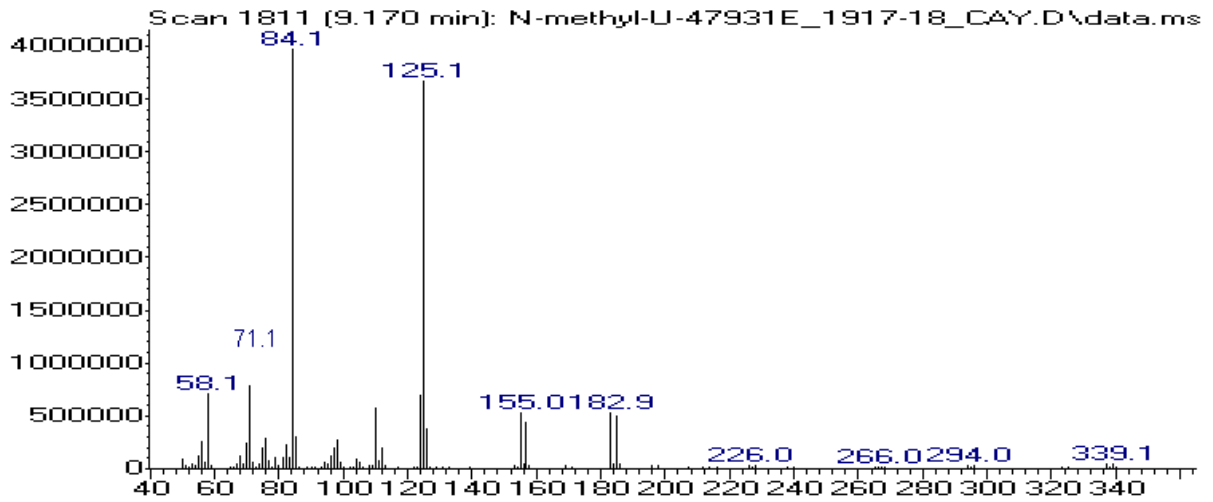
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

4. HPLC-TOF for exact monoisotopic mass and empirical formula control.

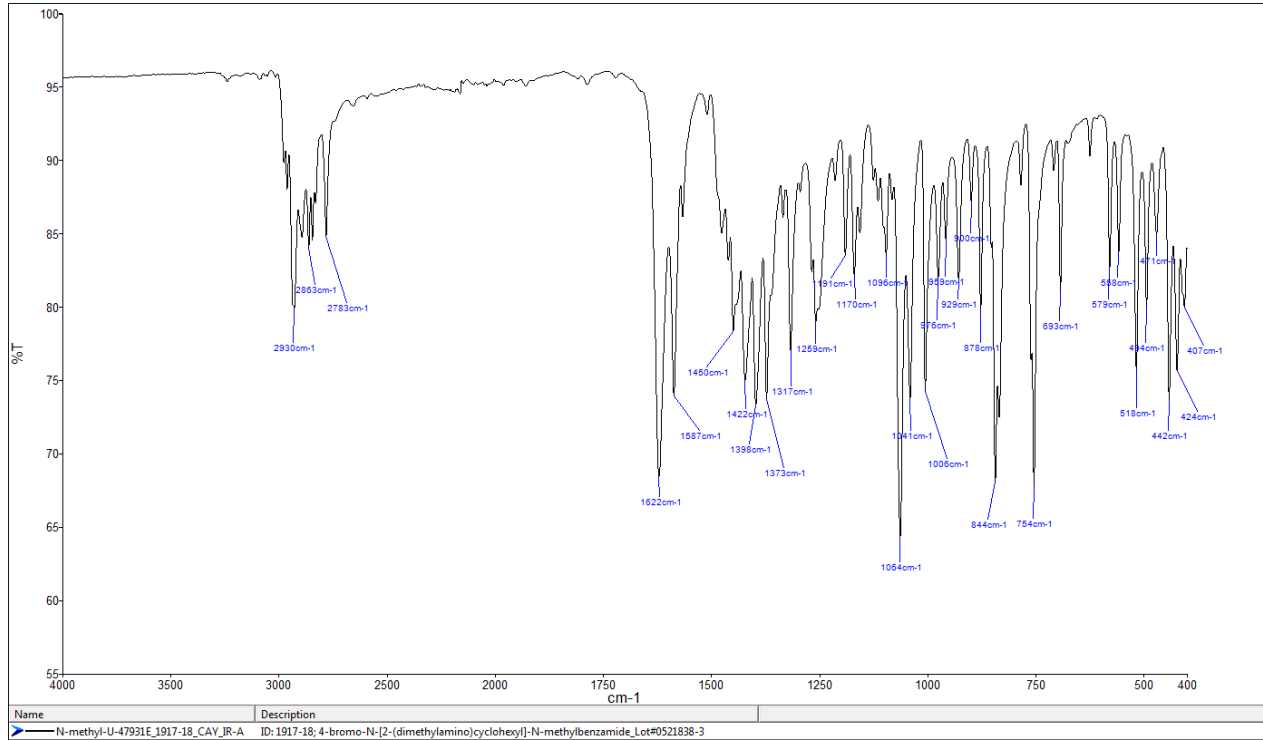
ANALYTICAL RESULTS

MS (EI)

Abundance



FTIR-ATR - sample as received



IR (condensed phase – after chromatographic separation)

