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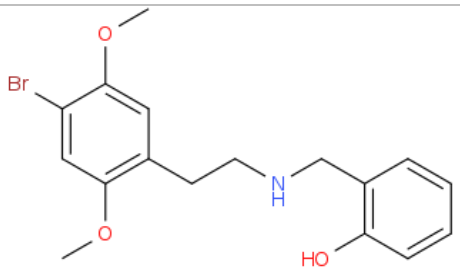
ANALYTICAL REPORT

25B-NBOH (C17H20BrNO3)

2-({[2-(4-bromo-2,5-dimethoxyphenyl)ethyl]amino}methyl)phenol

Remark – other active cpd. detected: none

Sample ID:	1700-16
Sample description:	powder - white
Sample type:	RM-reference material
Comments[1]:	CAY Lot#047570913; for GC-MS compound was derivatized by MSTFA: GC-RT and MS spectrum refer for di-TMS derivative; nonderivatized cpd. decomposed to 2C-BRESPONSE -purchasing
Date of entry:	1/5/2017

Substance identified-structure[2] (base form)	
Systematic name:	2-({[2-(4-bromo-2,5-dimethoxyphenyl)ethyl]amino}methyl)phenol
Other names:	2C-B-NBOH, NBOH-2C-B
Formula (per base form)	C17H20BrNO3
M_w (g/mol)	366,26
Salt form:	HCl
StdInChIKey (for base form)	RSUNJYKZRKIBNB-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	98%
REMARK	GC-MS data (RT and MS spectrum) from Cayman`s certificate corresponds to 2C-B

[1] This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

[2] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

	compound, which is the thermal decomposition product of 25B-NBOH.

Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 11,3 (*RT per di-TMS derivative*) BP(1): 179; BP(2): 280,BP(3) :73, **NOTE: non derivatized substance decomposes to 2C-B under our experimental conditions.**
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form

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 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 7.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}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 ^{0}C. Chromatographic separation as above **(1).**
Split MS : IR = 1 : 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1}.

4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

ANALYTICAL RESULTS WITH COMMENTS

Not derivatized compound 25B-NBOH (see structure at the first page) decomposes (see **Figure 1**) to 2C-B under our GC-MS conditions. The mass spectrum at the 5.8 minutes corresponds to 2C-B (2,5-dimethoxy-4-bromophenethylamine) - see **Figure 2.**

The same effect we observed for all compounds from the 25X-NBOH class.

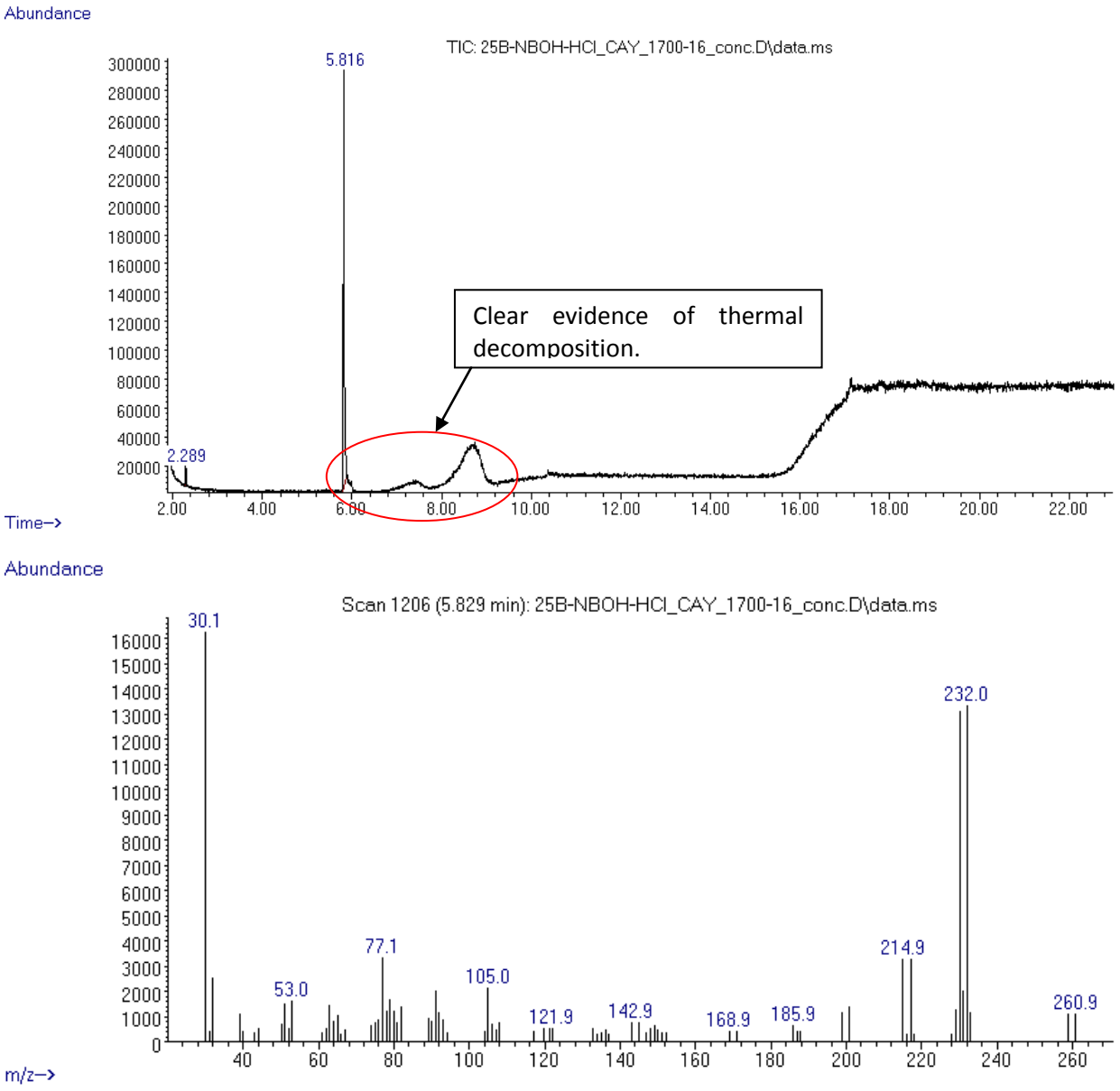


Figure 1: GC chromatogram of not derivatized sample (extract CH2Cl2 : MeOH in volume ratio 9 :1) and corresponding mass spectrum which fits with 2C-B spectrum from NIST(see below)

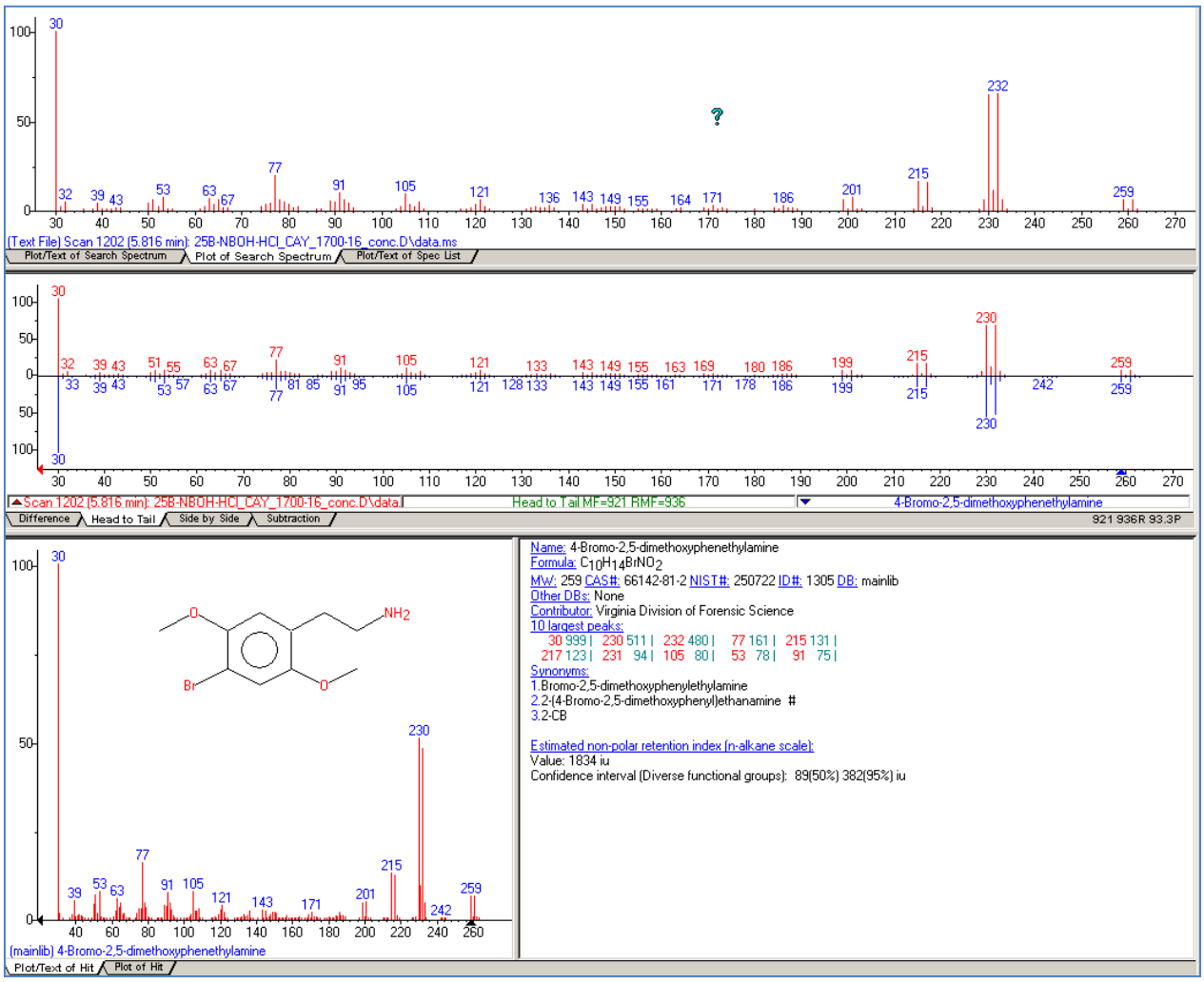


Figure 2: Experimentally observed spectrum at 5.2 min (red) is in agreement with NISTs 2C-B spectrum (blue).

In the next experiment the sample was dissolved in CHCL3 (approx. 0.8 ml) - pyridine (approx 0.1 ml) mixture and treated with 0.1 ml of MSTFA (N-Methyl-N-(trimethylsilyl) trifluoroacetamide derivatizing reagent for 20 min. at 70 ^{0}C.

The extract was analyzed by GC-MS. Chromatogram is shown on Figure 3, while mass spectra of 25B-NBOH-TMS and di-TMS derivatives are shown on figures Figure 5 and Figure 6, respectively.

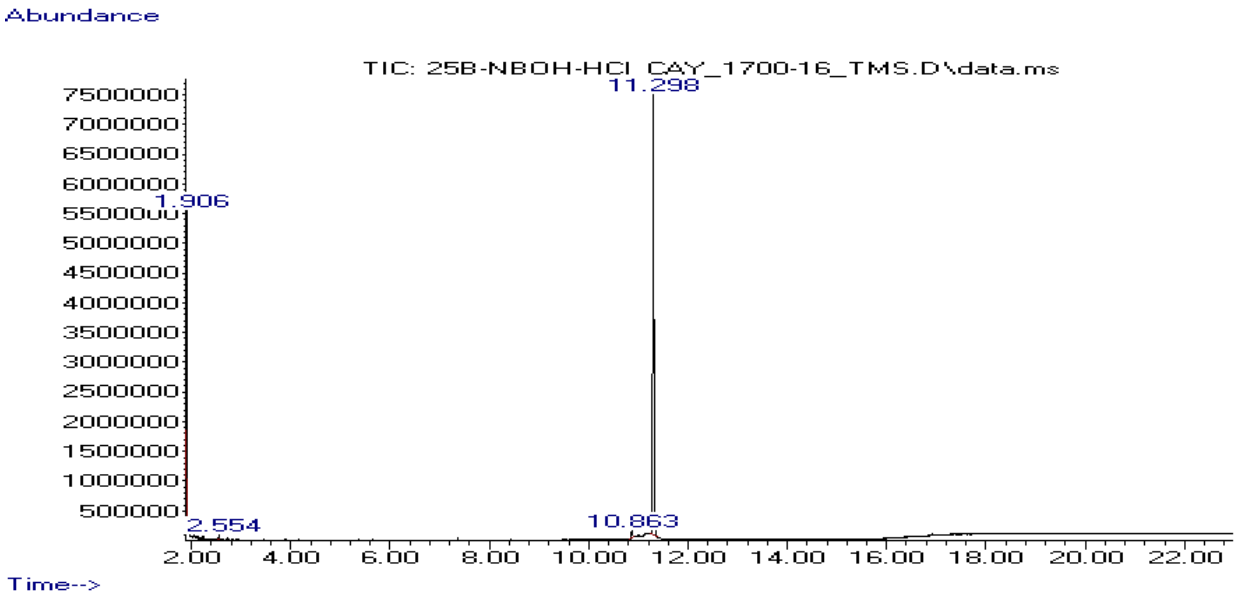


Figure 4: Chromatogram of TMS derivative. Small peak at 10.8 min corresponds to 25B-NBOH-TMS and peak at 11.3 to 25B-NBOH-di-TMS derivative.

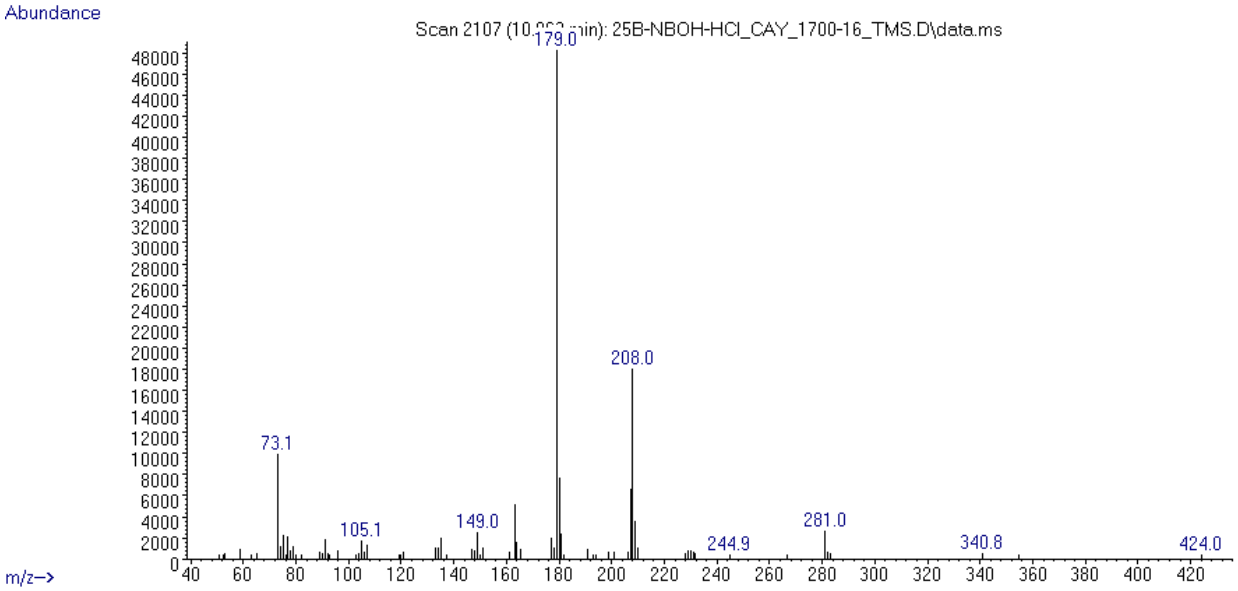


Figure 5: Mono-TMS derivative of the target compound

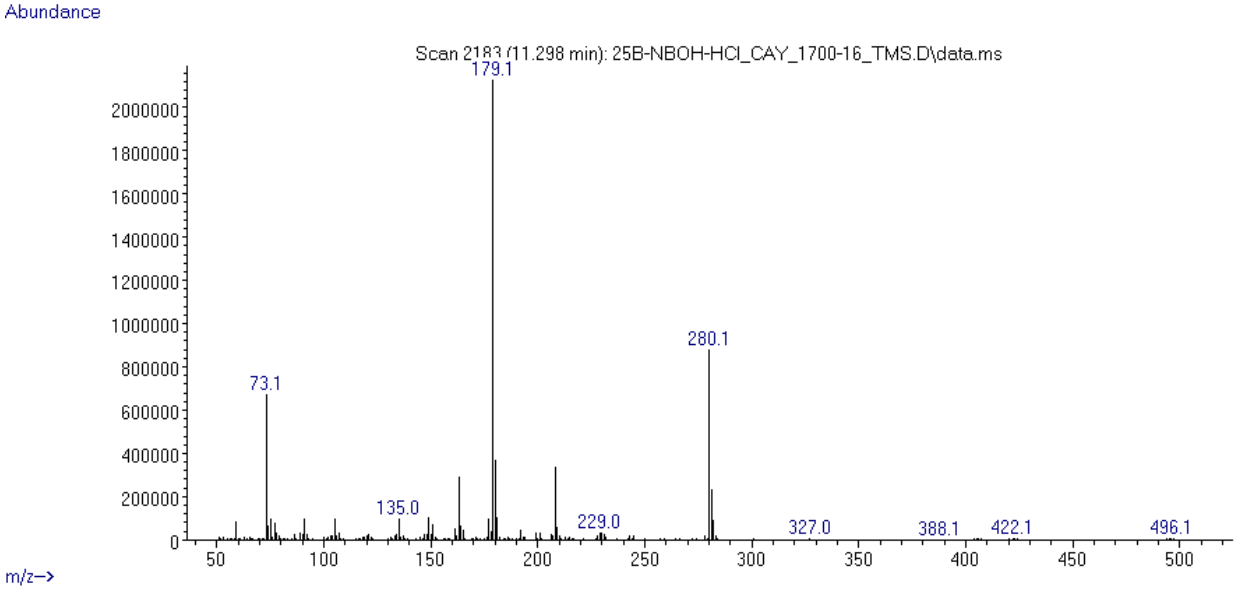


Figure 6:Di-TMS derivative of target compound

FTIR-ATR (sample as received)