

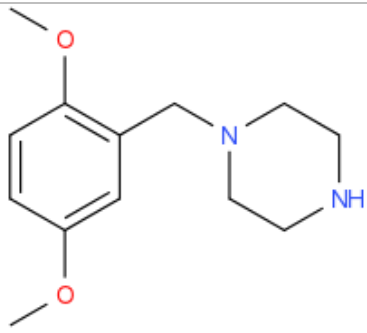
## ANALYTICAL REPORT

### 1-(2,5-Dimethoxybenzyl) piperazine (C<sub>13</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>)

#### 1-(2,5-Dimethoxybenzyl)piperazine

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

|                         |  |
|-------------------------|--|
| Sample ID:              | 1218-15                                  |
| Sample description:     | powder - white                           |
| Sample type:            | RM-reference material                    |
| Comments <sup>1</sup> : | Chiron AS Lot#15236 RESPONSE -purchasing |
| Date of entry:          | 8/31/2015                                |

|   |  |
|---|--|
| Substance identified-structure <sup>2</sup> (base form) |  |
| Systematic name:  | 1-(2,5-Dimethoxybenzyl)piperazine  |
| Other names:  |  |
| Formula (per base form)                                 | C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>                      |
| M <sub>w</sub> (g/mol)                                  | 236,32   |
| Salt form:  | HCl  |
| StdInChIKey   | KITIJFNTLBMQD-UHFFFAOYSA-N   |
| Compound Class  | Piperazine derivates   |
| Other active cpd. detected                              | none   |
| Add.info (purity..)                                     | 98,50%   |

<sup>1</sup> 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.

<sup>2</sup> 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): 6,58<br>BP(1): 151; BP(2): 194,BP(3) :121, |
| FTIR-ATR                | +       | direct measurement  |
| GC-IR (condensed phase) | +       | spectrum is always for the base form of compound            |

### 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 quadrupole 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<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

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.

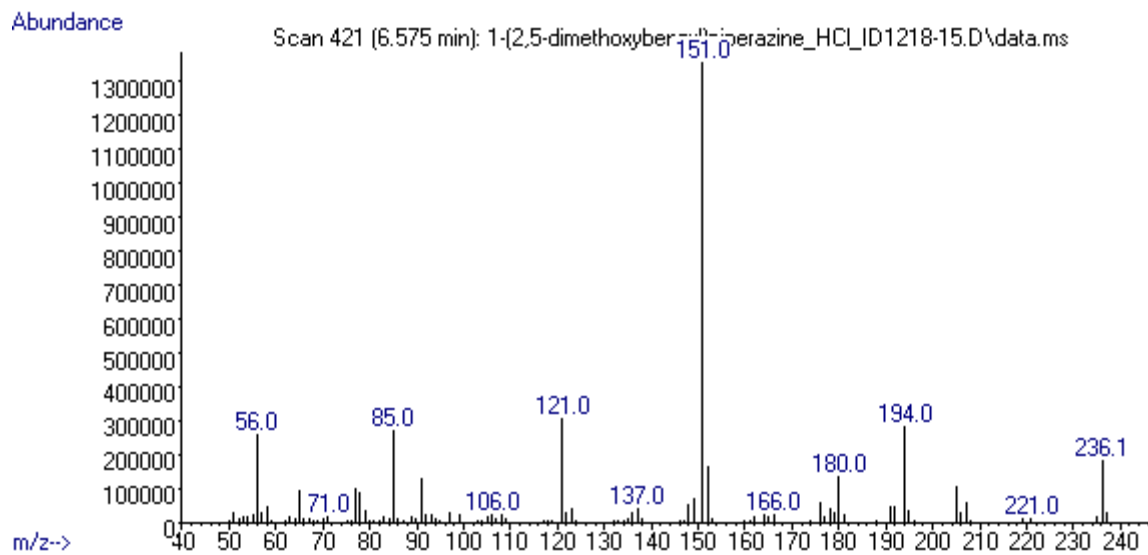
Split MS : IR : (1:9)

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

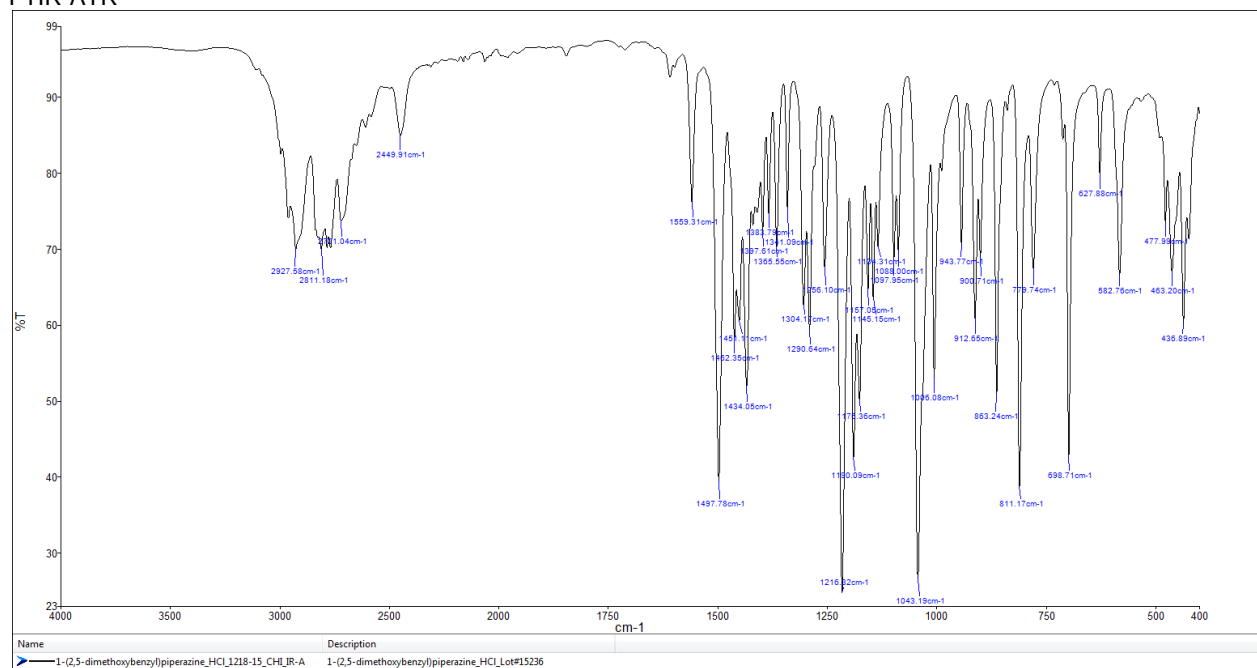
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

## FIGURES OF SPECTRA

MS (EI)



FTIR-ATR



## IR-condensed phase

