

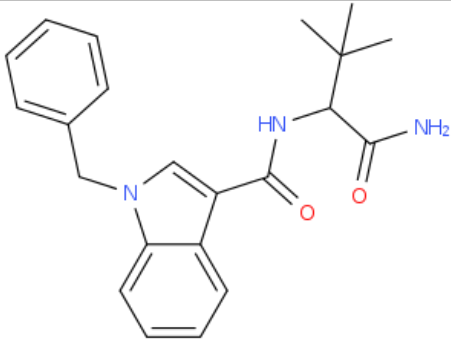
ANALYTICAL REPORT

ADB-BICA (C₂₂H₂₅N₃O₂)

2-[(1-benzyl-1H-indol-3-yl)formamido]-3,3-dimethylbutanamide

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

| | |
|-------------------------|---|
| Sample ID: | 1768-17 |
| Sample description: | powder - white-off |
| Sample type: | RM-reference material |
| Comments ¹ : | CAY Lot#0487299-8; RESPONSE -purchasing |
| Date of entry: | 3/9/2017 |

| | |
|---|--|
| Substance identified-structure ² (base form) |  |
| Systematic name: | 2-[(1-benzyl-1H-indol-3-yl)formamido]-3,3-dimethylbutanamide |
| Other names: | N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-benzyl-1H-indole-3-carboxamide |
| Formula (per base form) | C ₂₂ H ₂₅ N ₃ O ₂ |
| M _w (g/mol) | 363,46 |
| Salt form: | base |
| StdInChIKey (for base form) | OGVITAUBEIKNKNT-UHFFFAOYSA-N |
| Other active cpd. detected | none |
| Add.info (purity..) | 98% |

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



Report updates

| date | comments (explanation) |
|------|------------------------|
| | |
| | |
| | |
| | |

Supporting information

| Analytical technique: | applied | remarks |
|-------------------------|---------|--|
| GC-MS (EI ionization) | + | NFL GC-RT (min): 15,88 BP(1): 234; BP(2): 91,BP(3) :235, |
| 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 °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 quadropole 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 quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

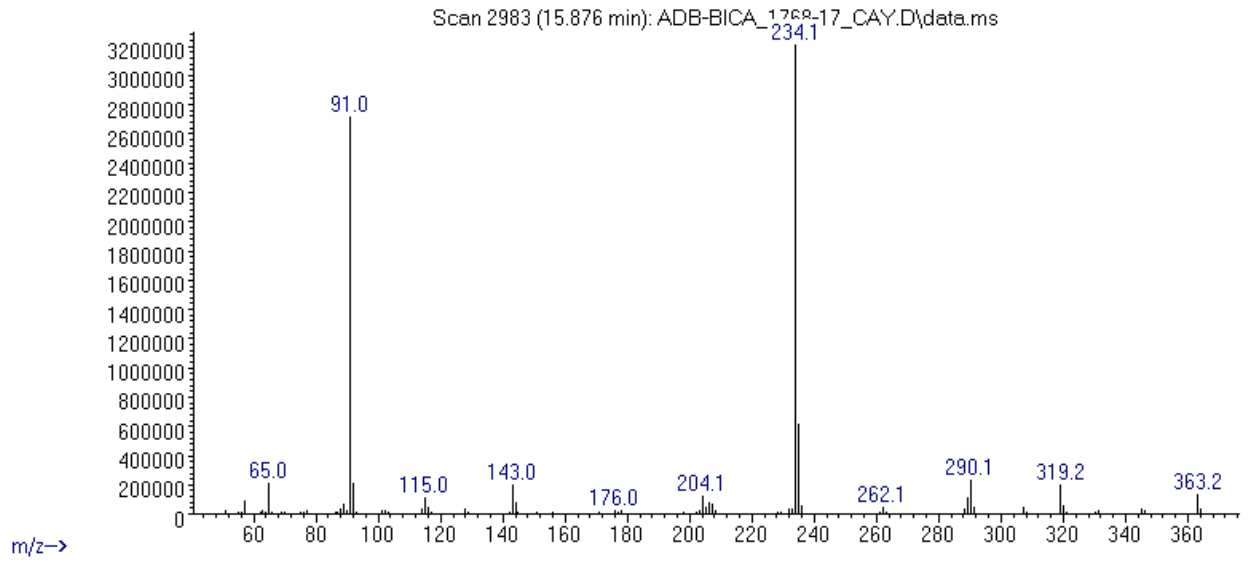
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

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

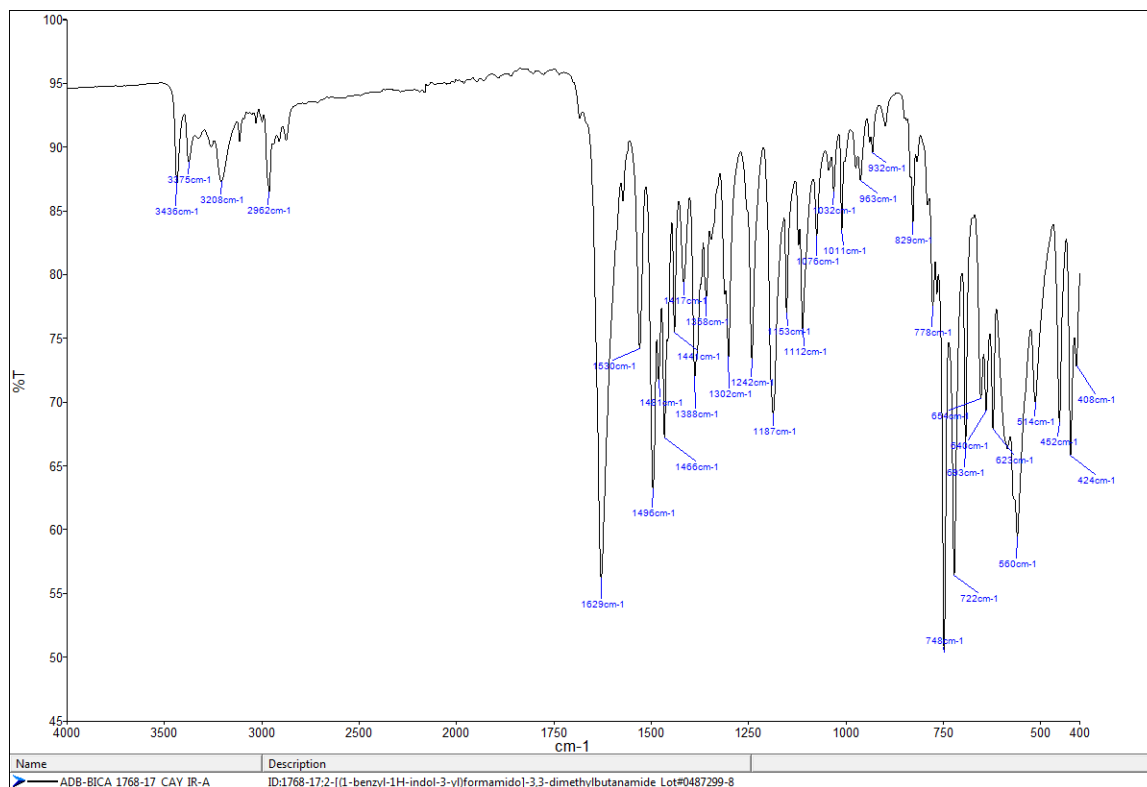
ANALYTICAL RESULTS

MS (EI)

Abundance



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)

