ANALYTICAL REPORT

APICA (C24H32N2O)

N-(adamantan-1-yl)-1-pentyl-1H-indole-3-carboxamide

Remark – other active cpd. detected: none

| Sample ID: | 1792-17 |
| Sample description: | powder - white |
| Sample type: | RM-reference material |
| Comments¹: | CHIRON Batch# 15 307; RESPONSE -purchasing |
| Date of entry: | 4/6/2017 |

Substance identified- structure² (base form)

![Chemical Structure](image)

Systematic name: N-(adamantan-1-yl)-1-pentyl-1H-indole-3-carboxamide

Other names: JWH-018 adamantyl carboxamide; 1-Pentyl-N-(tricyclo[3.3.1.13.7]dec-1-yl)-1H-indole-3-carboxamide; SDB 001; 2NE1

Formula (per base form) C24H32N2O

M₆ (g/mol) 364.53

Salt form: base

StdInChIKey (per base form) MDJYHWLDDJBTMX-UHFFFAOYSA-N

Other active cpd. detected none

Add.info (purity..) 99,7%

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/](http://opsin.ch.cam.ac.uk/) DOI: 10.1021/ci100384d
Supporting information

Analytical technique: | applied | remarks
---|---|---
GC-MS (EI ionization) | + | NFL GC-RT (min): 1,56 BP(1): 214; BP(2): 144, BP(3): 307,
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 El = 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 El = 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.
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

Scan 3102 (16.567 min) APICA_1792-17_CLIdatamecrs
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)

NOTE: This is condensed phase IR (per base form of substance) Instrument (Diavite GC-CC)