ANALYTICAL REPORT

JWH-122 (C25H25NO)

3-(4-methylnaphthalene-1-carbonyl)-1-pentyl-1H-indole

Remark – other active cpd. detected: none

Sample ID: 1489-16
Sample description: liquid - clear
Sample type: RM-reference material
Comments: LGC Lot#11998; I-SEE project RM and report
Date of entry: 5/12/2016

Substance identified- structure\(^2\) (base form)

Systematic name: 3-(4-methylnaphthalene-1-carbonyl)-1-pentyl-1H-indole
Other names: (4-Methyl-1-naphthyl)(1-pentyl-1H-indol-3-yl)methanone
Formula (per base form) C25H25NO
M\(_w\) (g/mol) 355.48
Salt form: base
StdInChIKey HUKJQMKQFWYIHS-UHFFFAOYSA-N
Compound Class Cannabinoids
Other active cpd. detected none
Add.info (purity..) 1 mg/ml in ACN

\(^1\) 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/6426). 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

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
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Supporting information

<table>
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<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 16.09 BP(1): 355; BP(2): 214, BP(3): 298,</td>
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<td>FTIR-ATR</td>
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<td>GC-IR (condensed phase)</td>
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**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, than 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 (30 until 6 min) to 550 (300) amu.

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

**GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny))** IR scan range 4000 to 700, resolution 4cm-1
- 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, than 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 (30 until 6 min) to 550 (300) amu.
- IR (condensed phase): IR scan range 4000 to 700, resolution 4cm-1
FIGURES OF SPECTRA

MS (EI)

Abundance

Scan 3:20 (t16, 380 min): LwH-122, 1439 16 D\data\.ms

m/z ->