# ANALYTICAL REPORT

## JWH-016 (C24H23NO)

### 1-butyl-2-methyl-3-(naphthalene-1-carbonyl)-1H-indole

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

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1882-17</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>powder - ligth yellow</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
</tr>
<tr>
<td>Comments:</td>
<td>Chiron AS Lot#11285,</td>
</tr>
<tr>
<td>Date of entry (DD/MM/YYYY):</td>
<td>04/12/2017</td>
</tr>
</tbody>
</table>

### Substance identified-structure\(^1\) (base form)

![Chemical Structure](image)

**Systematic name:** 1-butyl-2-methyl-3-(naphthalene-1-carbonyl)-1H-indole

**Other names:**
- (1-butyl-2-methyl-1H-indol-3-yl)-1-naphthenyl-methanon
- 1-Butyl-2-methyl-3-(1-naphthoyl)indole

**Formula (per base form):** C24H23NO

**M\(_w\) (g/mol):** 341.45

**Salt form:** base

**StdInChIKey (per base form):** QKXRHYJSCZFHEK-UHFFFAOYSA-N

**Other active cpd. detected:** none

**Add.info (purity..):** 99.2 %

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\(^1\) Created by OPSIN free tool: [http://opsin.ch.cam.ac.uk/](http://opsin.ch.cam.ac.uk/)  DOI: 10.1021/ci100384d
Report updates

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

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 14,3 BP(1): 341; BP(2): 127, BP(3): 340,</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
</tr>
<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td>always as base form</td>
</tr>
</tbody>
</table>

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))
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.
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.
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)