ANALYTICAL REPORT

NPB-22 (C22H21N3O2)

1-pentyl-1H-indazole-3-carboxylic acid, 8-quinolinyl ester

Remark – other active cpd. detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1423-15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>powder - white</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
</tr>
<tr>
<td>Comments¹:</td>
<td>Chiron AS Lot#15622; NFL- purchasing</td>
</tr>
<tr>
<td>Date of entry:</td>
<td>1/6/2016</td>
</tr>
</tbody>
</table>

Substance identified-structure² (base form)

![Structure Image]

Systematic name: 1-pentyl-1H-indazole-3-carboxylic acid, 8-quinolinyl ester

Other names: PB-22 indazole analogue

Formula (per base form) C22H21N3O2

Mₗ (g/mol) 359.43

Salt form: base

StdInChIKey UWICFJAXLKCHTQ-UHFFFAOYSA-N

Compound Class Cannabinoids

Other active cpd. detected none

Add.info (purity..) 98.90%

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

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13 April 2018</td>
<td>Mw typo error corrected</td>
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</table>

Supporting information

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
</tr>
</thead>
</table>
| GC-MS (EI ionization) | +       | NFL GC-RT (min): 15.25  
|                       |         | BP(1): 215; BP(2): 145,BP(3) :216, |
| FTIR-ATR              | +       | direct measurement |
| GC-IR (condensed phase) | +     |         |

**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 thickens 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 quadropole 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-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 thickens 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 quadropole 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-1
FIGURES OF SPECTRA

MS (EI)

Abundance

Scan 2873 (15.246 mn): NPB_22_1423-15_CHI_D\data.ms

m/z→

53.0  90.0  116.1  145.0  171.0  193.0  215.1  220  225.1  260.1  288.0  314.0  359.1
**FTIR-ATR**

![FTIR-ATR spectrum](image1)

**IR-Condensed phase**

![IR-Condensed phase spectrum](image2)

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFR_021213-15_1421_1</td>
<td>2-pentyl-6-quinolineketone 2H-indol-3-carboxylic acid</td>
</tr>
<tr>
<td>MFR_021213-15_1421_2</td>
<td>Sample 2-pentyl-6-quinolineketone 2H-indol-3-carboxylic acid</td>
</tr>
</tbody>
</table>

**Note:** This is condensed phase IR (per base form of substance) measurement (DisatIR-GC)