ANALYTICAL REPORT

FUB-NPB-22 (C24H16FN3O2)

quinolin-8-yl 1-(4-fluorobenzyl)-1H-indazole-3-carboxylate

Remark – other active cpd. detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1359-15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>crystalinic - white</td>
</tr>
<tr>
<td>Comments¹:</td>
<td>Cayman Lot#0464270; NFL- purchasing</td>
</tr>
<tr>
<td>Date of entry:</td>
<td>11/18/2015</td>
</tr>
</tbody>
</table>

Substance identified-structure² (base form)

![Substance structure](image-url)

Systematic name: quinolin-8-yl 1-(4-fluorobenzyl)-1H-indazole-3-carboxylate

Other names: 5-fluoro NIN; FUB-PB-22 indazole analog

Formula (per base form) C24H16FN3O2

M_w (g/mol) 397.4

Salt form: base

StdInChIKey NYHGKZZRRCVGAU-UHFFFAOYSA-N

Compound Class Cannabinoids

Other active cpd. detected none

Add.info (purity..) 95%

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

<table>
<thead>
<tr>
<th>Analytical technique</th>
<th>applied</th>
<th>remarks</th>
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</thead>
</table>
| GC-MS (EI ionization)        | +       | NFL GC-RT (min): 17.74
BP(1): 109; BP(2): 253, BP(3) : 254,                                    |
| 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