ANALYTICAL REPORT

CUMYL-5F-P7AICA, (C22H26FN3O)
1-(5-fluoropentyl)-N-(2-phenylpropan-2-yl)-7-azaindole-3-carboxamide

Remark – other NPS detected: none

Sample ID: 1154
Sample description: powder - white
Sample type: S-seized
Date of entry: 3/27/2015

Substance identified-structure (base form)

Systematic name 1-(5-fluoropentyl)-N-(2-phenylpropan-2-yl)-7-azaindole-3-carboxamide

Other names

Formula (per base form) C22H26FN3O
M_w (g/mol) 367,5
Salt form base
StdInChiKey MXJYOUJYNQPEY-UHFFFAOYSA-N

Compound Class Cannabinoids
Other NPS detected none
Add.info (purity..) Pure
Report updated: 13-Mar-16: “Smiles” code field was replaced by “StdInChiKey” code filed and code corrected.

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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>BP(1): 233; BP(2): 145; BP(3): 117,</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>FTIR (condensed phase)</td>
<td>/</td>
<td></td>
</tr>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
<td>formula:C22H26FN3O</td>
</tr>
<tr>
<td>NMR-confirmed</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>validation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>other</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**MS spectrum (El)**

![MS spectrum image]

Average of 12.829 to 12.867 min: CUMYL-5F-P7AICA_C-4245-800044-14.D\data.ms
FTIR - ATR

Name Description

*Created by OPSIN free tool: [http://opsin.ch.cam.ac.uk/](http://opsin.ch.cam.ac.uk/), DOI: 10.1021/ci100384d
**REPORT**

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>CARINA 4245-800044/2014</th>
</tr>
</thead>
<tbody>
<tr>
<td>Received date:</td>
<td>February 12, 2015</td>
</tr>
<tr>
<td>Our notebook code:</td>
<td>P-4245-800044-2014</td>
</tr>
<tr>
<td>NMR sample preparation:</td>
<td>5 mg dissolved in 0.7 mL CDCl₃</td>
</tr>
<tr>
<td>NMR experiments:</td>
<td>¹H, ¹³C</td>
</tr>
</tbody>
</table>

**Proposed structure with chemical name:**

```
  O
 N
    N
  \   / F
   \ /  \\
   F
```

1-(5-fluoropentyl)-N-(2-phenylpropan-2-yl)-¹H-pyrrolo[2,3-b]pyridine-3-carboxamide

**Comments:**
- Structure confirmed by ¹H and ¹³C NMR spectra.
- Compound is pure by NMR.

**Supporting information:** Copies of ¹H and ¹³C NMR spectra

**Author:** Prof. Dr. Janez Košmrlj

**Date of report:** February 14, 2015

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**Current Data Parameters**

**NAME** P-4245-800044-2014  
**EXPNO 1**  
**PROCNO 1**  

---

**F2 - Acquisition Parameters**

- Date: 20150214  
- Time: 6.26  
- INSTRUM: spect  
- PROBHD: 5 mm PABBO BB-  
- PULPROG: zg30  
- TD: 65536  
- SOLVENT: CDCl3  
- NS: 16  
- DS: 2  
- SWH: 10330.578 Hz  
- FIDRES: 0.157632 Hz  
- AQ: 3.1719923 sec  
- RG: 161  
- DW: 48.400 usec  
- DE: 6.50 usec  
- TE: 296.0 K  
- D1: 1.00000000 sec  

**======== CHANNEL f1 ========**

- NUC1: 1H  
- P1: 8.90 usec  
- PLW1: 26.00000000 W  
- SFO1: 500.1330885 MHz  

---

**F2 - Processing parameters**

- SI: 65536  
- SF: 500.1300132 MHz  
- WDW: EM  
- SSB: 0  
- LB: 0.30 Hz  
- GB: 0  
- PC: 1.00  

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**Current Data Parameters**

**NAME** P-4245-800044-2014  
**EXPNO 2**  
**PROCNO 1**  

---

**F2 - Acquisition Parameters**

- Date: 20150214  
- Time: 11.26  
- INSTRUM: spect  
- PROBHD: 5 mm PABBO BB-  
- PULPROG: zg30  
- TD: 65536  
- SOLVENT: CDCl3  
- NS: 8278  
- DS: 4  
- SWH: 29761.904 Hz  
- FIDRES: 0.454131 Hz  
- AQ: 1.1010548 sec  
- RG: 1620  
- DW: 16.800 usec  
- DE: 6.50 usec  
- TE: 296.0 K  
- D1: 1.00000000 sec  
- D11: 0.03000000 sec  

**======== CHANNEL f1 ========**

- NUC1: 13C  
- P1: 9.00 usec  
- PLW1: 122.00000000 W  
- SFO1: 125.7703637 MHz  

**======== CHANNEL f2 ========**

- CPDPRG2: waltz16  
- NUC2: 1H  
- PCPD2: 80.00 usec  
- PLW2: 26.00000000 W  
- PLW12: 0.32179001 W  
- PLW13: 0.20595001 W  
- SFO2: 500.1320005 MHz  

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**F2 - Processing parameters**

- SI: 32768  
- SF: 125.7577899 MHz  
- WDW: EM  
- SSB: 0  
- LB: 1.00 Hz  
- GB: 0  
- PC: 1.40