### ANALYTICAL REPORT

**5F-3,5-ADB-PFUPYCA (C21H28F2N4O2)**

2-[[1-(5-fluoropentyl)-3-(4-fluorophenyl)-1H-pyrazol-5-yl]formamido]-3,3-dimethylbutanamide

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

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample ID:</td>
<td>1765-17</td>
</tr>
<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>CAY Lot#0474365-5; RESPONSE -purchasing</td>
</tr>
<tr>
<td>Date of entry:</td>
<td>3/6/2017</td>
</tr>
</tbody>
</table>

#### Substance identified-structure² (base form)

![Chemical Structure](image)

**Systematic name:** 2-[[1-(5-fluoropentyl)-3-(4-fluorophenyl)-1H-pyrazol-5-yl]formamido]-3,3-dimethylbutanamide

**Other names:** ADB-FUPYCA; 3,5-5-fluoro ADB-FUPPYCA; AZ-037

**Formula (per base form):** C21H28F2N4O2  
**M_w (g/mol):** 406.48

**Salt form:** base

**StdInChIKey (for base form):** CMXMTA2Z3ECQ4-UHFFFAOYSA-N

**Other active cpd. detected:** none

**Add.info (purity..):** 98%

---

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
Report updates

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

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): 12,92 BP(1): 189; BP(2): 277, BP(3) :249,</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 thickens 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 0C 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.
ANALYTICAL RESULTS

MS (EI)

Scan 2465 (12.917 min) 5 3-5-ADB-PPGFYCA_1765-17_CAYDiDiata.ms

Abundance

m/z ->

69.1 95.0 134.0 162.0 221.0 249.1 277.1 333.1 362.1 406.2
FTIR-ATR - direct measurement (sample as received)

IR (condensed phase – after chromatographic separation)

NOTE: This is condensed phase IR (as base form of substance)
Instrument (DiscoFF-GC)

Name | Description
--- | ---
5-fluoro-3-[[N-[4-phenylphenyl]carbamoyl]amino]-2-(β-D-threopyranosyl)pyran-3-yl] (formamide) | 1,3-dimethylbutanamide, lot #0414385-5

Name | Description
--- | ---
5-[[N-[4-phenylphenyl]carbamoyl]amino]-2-(β-D-threopyranosyl)pyran-3-yl] (formamide) | 1,3-dimethylbutanamide, lot #0414385-5