ANALYTICAL REPORT

AMB-CHMINACA (C21H29N3O3)

methyl 2-[[1-(cyclohexylmethyl)-1H-indazol-3-yl]formamido]-3-methylbutanoate

Remark – other active cpd. detected: none

Sample ID: 1790-17
Sample description: liquid - colorless
Sample type: RM-reference material
Comments: CHIRON Batch# 15 799; RESPONSE -purchasing
Date of entry: 3/31/2017

Substance identified-structure (base form)

Systematic name: methyl 2-[[1-(cyclohexylmethyl)-1H-indazol-3-yl]formamido]-3-methylbutanoate

Other names: Methyl 2-((1-(cyclohexylmethyl)-1H-indazole-3-carboxamide)-3-methylbutanoate; MA-CHMINACA; AMB N-methyl/cyclohexyl analog; MAB-AB-CHMINACA

Formula (per base form) C21H29N3O3
M_w (g/mol) 371,48
Salt form: base
StdInChIKey (for base form) CRGXDSTBHQLKJ-UHFFFAOYSA-N
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/ DOI: 10.1021/ci100384d
Report updates

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

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 11,65 BP(1): 241; BP(2): 145, BP(3): 312,</td>
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<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td>always as base form</td>
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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 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 El = 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 4 cm⁻¹

3. **GC-MS**-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
MSD source El = 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)

Abundance

Scn 2244 [11.647 min]: AMB-CHMINAC=+

m/z -->
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)