# ANALYTICAL REPORT

**MDMB-INACA (C15H19N3O3)**

methyl 2-[(1H-indazol-3-yl)formamido]-3,3-dimethylbutanoate

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

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>2074-19</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description</td>
<td>powder - white</td>
</tr>
<tr>
<td>Sample type</td>
<td>RM-reference material</td>
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<tr>
<td>Comments</td>
<td>CAY Lot#0552665-3,</td>
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<tr>
<td>Date of entry</td>
<td>28/06/2019</td>
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</tbody>
</table>

## Substance identified-structure\(^1\) (base form)

\[\text{methyl 2-[(1H-indazol-3-yl)formamido]-3,3-dimethylbutanoate}\]

## Systematic name

methyl 2-[(1H-indazol-3-yl)formamido]-3,3-dimethylbutanoate

## Other names

methyl 2-(1H-indazole-3-carboxamido)-3,3-dimethylbutanoate

## Formula (per base form)

C15H19N3O3

## M\(_w\) (g/mol)

289,33

## Salt form

base

## StdInChIKey (per base form)

QEXPVGOZJEEO-UHFFFAOYSA-N

## Other active cpd. detected

none

## Add.info (purity..)

\(\geq 98\%\)

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\(^1\) 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>
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<tbody>
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Supporting information

Analytical technique: | applied | remarks
---|---|---
GC-MS (EI ionization) | + | NFL GC-RT (min): 9.47 BP(1): 145; BP(2): 201, BP(3): 233, FTIR-ATR | + | direct measurement
GC-IR (condensed phase) | + | always as base form
HPLC-TOF | + | exact mass theoretical: 289,1426 / measured Δppm: -1.17

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 °C 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 4 cm⁻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) amu.
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

4. **HPLC-TOF** (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.
ANALYTICAL RESULTS

MS (EI)

Abundance

Scan 1863 (3.457 min): MOMBINACA_2074-18_CAY_Dadato.ms

145.0

57.1

201.1

233.1

m/z →

3

Stran 3 od 4

ID 2074-19
FTIR-ATR – direct measurement

IR- (condensed (solid) phase – after chromatographic separation) - spectrum per base form

NOTE: This is condensed phase IR (per base form of substance)