ANALYTICAL REPORT

4,5-MDAI (C10H11NO2)

2H,6H,7H,8H-indeno[4,5-d][1,3]dioxol-7-amine

Remark – other active cpd. detected: none

Sample ID: 1877-17
Sample description: powder - white
Sample type: RM-reference material
Comments: CAY Lot#0505225-3,
Date of entry (DD/MM/YYYY): 10/11/2017

Substance identified-structure1 (base form)

Systematic name: 2H,6H,7H,8H-indeno[4,5-d][1,3]dioxol-7-amine
Other names: 7,8-dihydro-6H-indeno[4,5-d]-1,3-dioxol-7-amine
Formula (per base form): C10H11NO2
Mw (g/mol): 177,2
Salt form: HCl
StdInChIKey (per base form): AHYFDWHTTFREHS-UHFFFAOYSA-N
Other active cpd. detected: none
Add.info (purity..): 99,2 %

1 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>
</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): 4,35 BP(1): 177; BP(2): 160, BP(3): 149,</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>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
<td>exact monoisotopic mass: 177,079 (\Delta ppm) (difference from calculated): 2,3</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 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 El = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole 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 El = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole 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 (see the table above)
ANALYTICAL RESULTS

MS (EI)

Scan 754 (4.351 min), 4-5-MDAI_CAY_1877-17.Dijdata.ms

m/z→

30.1  51.1  77.0  91.1  105.0  118.1  135.0  160.0  177.1  206.3

Abundance
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)