ANALYTICAL REPORT

4-AcO-DPT (C18H26N2O2)

3-[2-(dipropylamino)ethyl]-1H-indol-4-yl acetate

Remark – other active cpd. detected: none

Sample ID: 1916-18
Sample description: powder - yellow
Sample type: RM-reference material
Comments: CAY Lot#0516586-4,
Date of entry (DD/MM/YYYY): 09/04/2018

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

Systematic name: 3-[2-(dipropylamino)ethyl]-1H-indol-4-yl acetate
Other names: 4-acetoxy-N,N-Dipropyltryptamine; 4-AcO-DPT; 4-acetoxy DPT
Formula (per base form) C18H26N2O2
M\(_w\) (g/mol) 302,42
Salt form: acetate
StdInChIKey (per base form) KRUGABVNNKKCJN-UHFFFAOYSA-N
Other active cpd. detected none
Add.info (purity..) \(\geq 95\%\)

\(^1\) 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>
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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>NFL GC-RT (min): 9,35 BP(1): 114; BP(2): 115,BP(3):86,</td>
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<tr>
<td>FTIR-ATR</td>
<td>direct measurement</td>
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<td>GC-IR (condensed phase)</td>
<td>always as base form</td>
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<tr>
<td>HPLC-TOF</td>
<td>exact monoisotopic mass: 302.1994 ∆ppm (difference from calculated): 0,72</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 0C. 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 0C for 1 min, followed by heating up to 190 0C at rate 8 0C/min, then heating up to 293 0C at a rate of 18 0C/min, hold for 7.1 min, then heating at 50 0C/min up to 325 0C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 2350C, source and quadropole temperatures 2800C and 1800C, 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)
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 0C. Chromatographic separation as above (1). Split MS: IR = 1 : 9. MSD source EI = 70 eV. GC-MS transfer line T= 2350C, source and quadropole temperatures 2800C and 1800C, 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
ANALYTICAL RESULTS

MS (EI)
Abundance

Stran 1842 (9.347 min) 4-AcO-DPT_1916-18_CAYD_data.ms
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)