Datasheet Diethylstilbestrol-D₆

Reference number : CEC/MAT : 01

Date of preparation: 1993.01.29

date : 29 November 2002

source : RIVM

“Bank of Reference Standards”

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Contract MAT 1 - CT92 - 0020
Name: (E)-4,4’-[(1,2-di-(1’,1’,1’-trideuterio)ethyl)-1,2-ethenediy]bisphenol
Synonym: trans-diethylstilbestrol-D_6
Molecular formula: C_{18}H_{14}D_{6}O_{2}
Cas #: 89717-83-9
Molecular weight: 274.4

Long term stability tested on 1997.09.03: 95.1 ± 0.3 %
(Storage 4°C, analysis HPLC-UV, 6 tests on 2 ampoules)

Last update: 1998.01.06

Methods used for characterization:

I  IR spectroscopy
II  Mass spectrometry
III HPLC-UV spectroscopy
IV  ^1H-NMR spectrometry
V   Homogeneity and stability obtained with GC-MS
I  IR-SPECTROSCOPY

Instrument: Bruker IFS-55 FTIR; detector DTGS
Sampling technique: KBr-tablet

II  MASS-SPECTROMETRY

Instrument: Hewlett Packard 5989 A MS
MS spectrum, DIP = direct inlet probe
III HPLC-UV SPECROSCOPY

Instrument: TSP spectrasystem UV2000; resolution 2nm.
HPLC eluens: methanol/water (70:30 v/v)
HPLC column: Lichrocart 125-4 hplc cartridge

IV $^1$H-NMR SPECTROMETRY

Instrument: FT-NMR Jeol GSX; 270 MHz, 5 mm probe, solvent CDCl$_3$

<table>
<thead>
<tr>
<th>Chemical shifts (ppm)</th>
<th>Amount of protons (multiplicity)</th>
<th>Designation</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.11</td>
<td>4 (m)</td>
<td>CD$_3$CH$_2$</td>
</tr>
<tr>
<td>6.95</td>
<td>8 (m)</td>
<td>arom.</td>
</tr>
</tbody>
</table>

* ethanol was found (1.1 en 3.6 ppm), used as solvent during ampouling.
V HOMOGENEITY AND STABILITY

**Stability and homogeneity test of DES-D₆**

**CEC/MAT: 01**

<table>
<thead>
<tr>
<th>Temp.</th>
<th>t = 0 months</th>
<th>t = 1, 5 months</th>
<th>t = 3 months</th>
<th>t = 6 months</th>
<th>t = 12 months</th>
<th>t = 24 months</th>
</tr>
</thead>
<tbody>
<tr>
<td>4°C</td>
<td>(99 ± 3)</td>
<td>(97 ± 1)</td>
<td>(98 ± 3)</td>
<td>(100 ± 3)</td>
<td>(106 ± 4)</td>
<td>(98 ± 2)</td>
</tr>
<tr>
<td>20°C</td>
<td>(96 ± 1)</td>
<td>(96 ± 3)</td>
<td>(103 ± 1)</td>
<td>(105 ± 1)</td>
<td>(94 ± 3)</td>
<td>(94 ± 3)</td>
</tr>
<tr>
<td>37°C</td>
<td>(97 ± 1)</td>
<td>(97 ± 1)</td>
<td>(99 ± 3)</td>
<td>(105 ± 1)</td>
<td>(96 ± 4)</td>
<td>(96 ± 4)</td>
</tr>
</tbody>
</table>

**Stability test Diethylstilbestrol-d6**

![Graph showing stability test results](image-url)