1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_{15}\text{H}_{17}\text{NO}_{2}\text{S}_{3} \cdot \frac{1}{4}\text{H}_{2}\text{O}$

Batch Molecular Weight: 344

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Ethyl acetate: Petroleum ether [2:3])

HPLC: Shows 99.3% purity

$^1$H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>52.38</td>
<td>52.17</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.13</td>
<td>4.99</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>4.07</td>
<td>3.99</td>
</tr>
</tbody>
</table>
Product Name: TB 21007

CAS Number: 207306-50-1

IUPAC Name: 6,7-Dihydro-3-[(2-hydroxyethyl)thio]-6,6-dimethyl-1-(2-thiazolyl)-benzo[c]thiophen-4(5H)-one

Description:
GABA<sub>α</sub> receptor inverse agonist selective for the α<sub>5</sub>-subtype (K<sub>i</sub> values are 1.6, 16, 20 and 20 nM for α<sub>5</sub>, α<sub>2</sub>, α<sub>1</sub> and α<sub>3</sub> subtypes respectively). Brain penetrant; enhances cognitive performance in rats in the delayed matching-to-place morris water maze test following i.p. administration.

Physical and Chemical Properties:
Batch Molecular Formula: C<sub>12</sub>H<sub>17</sub>NO<sub>3</sub>S<sub>3</sub>/4H<sub>2</sub>O
Batch Molecular Weight: 344
Physical Appearance: Off-white solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 25 mM

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References: