

## Certificate of Analysis

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**Product Name:** TB 21007

**Catalog No.:** 2905

**Batch No.:** 2

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

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>15</sub>H<sub>17</sub>NO<sub>2</sub>S<sub>3</sub>·¼H<sub>2</sub>O

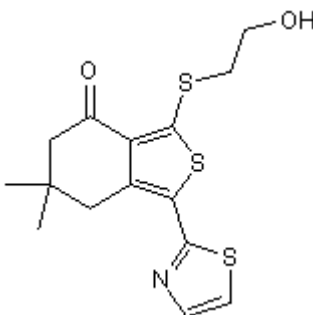
**Batch Molecular Weight:** 344

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 100 mM  
ethanol to 25 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.3 (Ethyl acetate:Petroleum ether [2:3])

**HPLC:** Shows 99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	52.38	5.13	4.07
Found	52.17	4.99	3.99

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**Description:**

GABA<sub>A</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:**

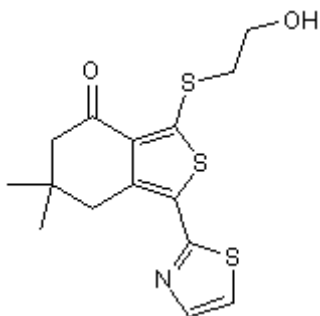
Batch Molecular Formula: C<sub>15</sub>H<sub>17</sub>NO<sub>2</sub>S<sub>3</sub> · ¼H<sub>2</sub>O

Batch Molecular Weight: 344

Physical Appearance: Off-white solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Chambers et al** (2003) Identification of a novel, selective GABA<sub>5</sub> α<sub>5</sub> receptor inverse agonist which enhances cognition. *J. Med. Chem.* **46** 2227. PMID: 12747794.

**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.

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