



Certificate of Analysis

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Tiagabine hydrochloride Catalog No.: 4256 Batch No.: 1 **Product Name:**

145821-59-6 CAS Number:

IUPAC Name: (3R)-1-[4,4-Bis(3-methyl-2-thienyl)-3-butenyl]-3-piperidinecarboxylic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

C₂₀H₂₅NO₂S₂.HCI.0.67H₂O **Batch Molecular Formula:**

Batch Molecular Weight: 424.02

Physical Appearance: Off-white solid water to 50 mM Solubility:

DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: Between 190 - 195°C HPLC: Shows 100% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -11.6 (Concentration = 1, Solvent = Water)

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 56.67 6.5 3.3 Found 56.68 6.14 3.34



Product Information

Print Date: Oct 11th 2024

1

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Description:

Tiagabine hydrochloride is a GABA uptake inhibitor ($IC_{50} = 67$ nM in vivo). Exhibits high affinity and selectivity for the GAT-1 GABA transporter. Anticonvulsant; also attenuates established dynorphin-induced allodynia in a mouse model after systemic administration.

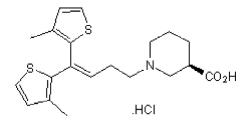
Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₂₅NO₂S₂.HCl.0.67H₂O

Batch Molecular Weight: 424.02 Physical Appearance: Off-white solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 50 mM DMSO to 100 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).

Catalog No.: 4256

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Laughlin *et al* (2002) Comparison of antiepileptic drugs tiagabine, lamotrigine, and gabap. in mouse models of acute, prolonged, and chronic nociception. J.Pharmacol.Exp.Ther. *302* 1168. PMID: 12183677.

Dhar *et al* (1994) Design, synthesis and evaluation of substituted triarylnipecotic acid derivatives as GABA updake inhibitors: identification of a ligand with moderate affinity and selectivity for the cloned human GABA transporter GAT-3. J.Med.Chem. *37* 2334. PMID: 8057281.

Andersen *et al* (1993) The synthesis of novel GABA uptake inhibitors. 1. Elucidation of the structure-activity studies leading to the choice of (R)-1-[4,4-bis(3-methyl-2-thienyl)-3-butenyl]-3-piperidinecarboxylic acid (tiagabine) as an anticonvulsant drug ca J.Med.Chem. **36** 1716. PMID: 8510100.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use