

Certificate of Analysis

Product Name: Tiagabine hydrochloride

Catalog No.: 4256

Batch No.: 1

CAS Number: 145821-59-6

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₅NO₂S₂·HCl·0.67H₂O

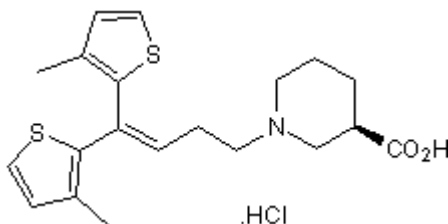
Batch Molecular Weight: 424.02

Physical Appearance: Off-white solid

Solubility: water to 50 mM
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: [α]_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

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

Product Name: Tiagabine hydrochloride

Catalog No.: 4256

Batch No.: 1

CAS Number: 145821-59-6

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

Description:

GABA uptake inhibitor (IC₅₀ = 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:

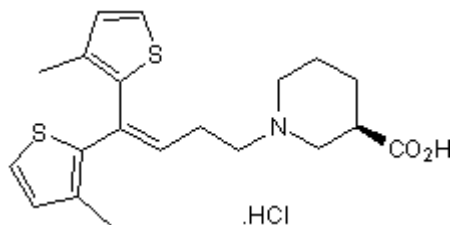
Batch Molecular Formula: C₂₀H₂₅NO₂S₂.HCl.O.67H₂O

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).

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:

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 candidate. *J.Med.Chem.* **36** 1716. PMID: 8510100.

Dhar et al (1994) Design, synthesis and evaluation of substituted triarylpipecotic acid derivatives as GABA uptake 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.

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

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956