

Certificate of Analysis

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Product Name: TCS 401

Catalog No.: 2754

Batch No.: 6

CAS Number: 243966-09-8

IUPAC Name: 2-[(Carboxycarbonyl)amino]-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₀H₁₀N₂O₅S.HCl.¾H₂O

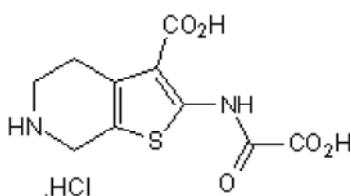
Batch Molecular Weight: 320.23

Physical Appearance: Beige solid

Solubility: 100mM NaOH to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical	37.51	3.93	8.75
Found	37.63	4.17	8.4

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

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Product Information

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IUPAC Name: 2-[(Carboxycarbonyl)amino]-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acid hydrochloride

Description:

Selective inhibitor of protein-tyrosine phosphatase 1B (PTP1B) (K_i values are 0.29, 59, 560, 1100, > 2000, > 2000 and > 2000 μ M for PTP1B, CD45 D1D2, PTP β , PTP ϵ D1, SHP-1, PTP α D1 and LAR D1D2 respectively).

Physical and Chemical Properties:

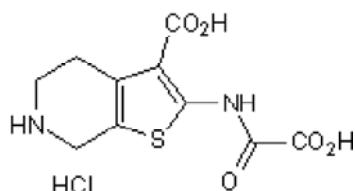
Batch Molecular Formula: C₁₀H₁₀N₂O₅S.HCl.¾H₂O

Batch Molecular Weight: 320.23

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

100mM NaOH to 20 mM

CAUTION - This product has been shown to be unstable in basic aqueous solutions. Therefore, we recommend that solutions should be made up and used within 24 hours

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 (2002) Discovery and SAR of a novel selective and orally bioavailable nonpeptide classical competitive inhibitor class of protein-tyrosine phosphatase 1B. *J.Med.Chem.* **45** 4443. PMID: 12238924.

Iversen et al (2000) Structure-based design of a low molecular weight, nonphosphorus, nonpeptide, and highly selective inhibitor of protein-tyrosine phosphatase 1B. *J.Biol.Chem.* **275** 10300. PMID: 10744717.

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