

Certificate of Analysis

Print Date: Feb 11th 2019

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Product Name: Thiamet G Catalog No.: 4390 Batch No.: 6

CAS Number: 1009816-48-1

 $(3aR, 5R, 6S, 7R, 7aR) - 2 - (Ethylamino) - 3a, 6, 7, 7a - tetrahydro - 5 - (hydroxymethyl) - 5H - pyrano[3, 2-d] \\ thiazole - 6, 7 - diologous - 6, 7 - diologous$ **IUPAC Name:**

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_9H_{16}N_2O_4S.^3/_4H_2O$ **Batch Molecular Formula:**

Batch Molecular Weight: 261.81 **Physical Appearance:** White solid

DMSO to 50 mM Solubility: Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

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

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 41.29 6.74 10.7 Found 41.42 6.55 10.68

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

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Product Information

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CAS Number: 1009816-48-1

IUPAC Name: (3aR,5R,6S,7R,7aR)-2-(Ethylamino)-3a,6,7,7a-tetrahydro-5-(hydroxymethyl)-5H-pyrano[3,2-d]thiazole-6,7-diol

Description:

Potent, selective inhibitor of O-GlcNAcase ($K_i = 21 \text{ nM}$ for human O-GlcNAcase). Decreases the phosphorylation of tau protein in vivo. Promotes autophagy independently of mTOR pathway and reduces toxic protein species in mouse tauopathy model. Orally bioavailable and blood brain barrier permeable.

Physical and Chemical Properties:

Batch Molecular Formula: C₉H₁₆N₂O₄S.³/₄H₂O

Batch Molecular Weight: 261.81 Physical Appearance: White solid

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Zhu et al (2018) Pharmacological inhibition of O-GlcNAcase enhances autophagy in brain through an mTOR-independent pathway ACS Chem.Neurosci. **9** 1366. PMID: 29460617.

Yuzwa et al (2008) A potent mechanism-inspired O-GlcNAcase inhibitor that blocks phosphorylation of tau in vivo. Nat.Chem.Biol. 4 483. PMID: 18587388.

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