

**Product Name:** ST 045849

**Catalog No.:** 6775

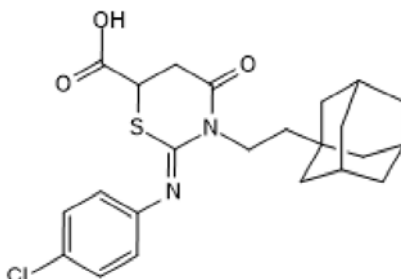
**Batch No.:** 1

CAS Number: 442665-87-4

IUPAC Name: 2-[(4-Chlorophenyl)imino]tetrahydro-4-oxo-3-(2-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-ylethyl)-2H-1,3-thiazine-6-carboxylic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>27</sub>ClN<sub>2</sub>O<sub>3</sub>S  
**Batch Molecular Weight:** 446.99  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 100 mM  
ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.2% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.8	6.09	6.27
Found	61.37	6.08	6.3

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

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**Description:**

O-GlcNAc transferase (OGT) inhibitor ( $IC_{50}$  = 53  $\mu$ M). Reduces proliferation and viability of prostate cancer cells in vitro. Depletes intracellular alanine and decreases glucose consumption by cancer cells. Decreases markers of ER stress and apoptosis in pregnant diabetic mice and reduces neural tube defects in embryos from diabetic mice.

**Physical and Chemical Properties:**

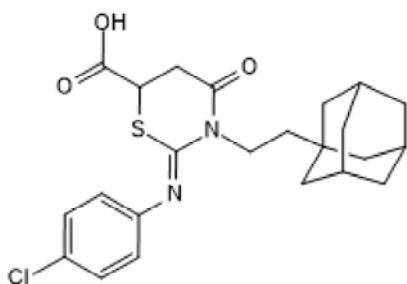
Batch Molecular Formula: C<sub>23</sub>H<sub>27</sub>ClN<sub>2</sub>O<sub>3</sub>S

Batch Molecular Weight: 446.99

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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:**

**Kim et al** (2017) Impact of protein O-GlcNAcylation on neural tube malformation in diabetic embryopathy. *Sci.Rep.* **7** 11107. PMID: 28894244.

**Itkonen et al** (2016) Inhibition of O-GlcNAc transferase activity reprograms prostate cancer cell metabolism. *Oncotarget* **7** 12464. PMID: 26824323.

**Kim et al** (2014) Versatile O-GlcNAc transferase assay for high-throughput identification of enzyme variants, substrates, and inhibitors. *Bioconjug.Chem.* **25** 1025. PMID: 24866374.

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