

**Product Name:** 

# **Certificate of Analysis**

Print Date: Oct 21st 2022

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Catalog No.: 3625 Batch No.: 4

CAS Number: 958772-66-2

IUPAC Name: N-[(1,1-Dimethylethoxy)carbonyl]-L-tryptophan-2-[[[2-[(2-ethylphenyl)amino]-2-oxoethyl]thio]carbonyl]hydrazide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

SID 26681509

**Batch Molecular Formula:**  $C_{27}H_{33}N_5O_5S$ 

**Batch Molecular Weight:** 539.65 **Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM

ethanol to 10 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 98.5% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -17$  (Concentration = 0.5, Solvent = Acetic Acid)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.09 6.16 12.98 Found 59.6 6.14 12.82

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## **Product Information**

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 $IUPAC\ Name: \ N-[(1,1-Dimethylethoxy)carbonyl]-L-tryptophan-2-[[[2-[(2-ethylphenyl)amino]-2-oxoethyl]thio]carbonyl] hydrazide$ 

#### **Description:**

SID 26681509 is a potent and reversible human cathepsin L inhibitor ( $IC_{50} = 56$  nM). Displays no inhibitory activity at cathepsin G. Antimalarial; inhibits leishmaniasis.

### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>27</sub>H<sub>33</sub>N<sub>5</sub>O<sub>5</sub>S Batch Molecular Weight: 539.65

Physical Appearance: White solid

### Minimum Purity: ≥97%

### **Batch Molecular Structure:**

Storage: Store at -20°C

### Solubility & Usage Info:

DMSO to 50 mM ethanol to 10 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:

Myers et al (2008) Identification and synthesis of a unique thiocarbazate cathepsin L inhibitor. Bioorg.Med.Chem.Lett. 18 210. PMID: 18060772.

**Shah** et al (2008) Kinetic characterization and molecular docking of a novel, potent and selective slow-binding inhibitor of human cathepsin L. Mol.Pharmacol. **74** 34. PMID: 18403718.

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