

Certificate of Analysis

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Product Name: LOC14

Catalog No.: 5606

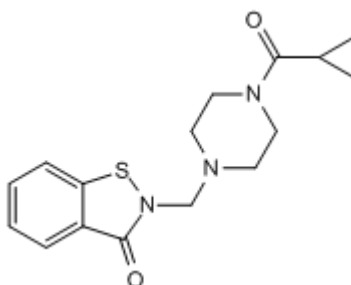
Batch No.: 1

CAS Number: 877963-94-5

IUPAC Name: 2-[[4-(Cyclopropylcarbonyl)-1-piperazinyl]methyl]-1,2-benzisothiazol-3(2H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₉N₃O₂S
Batch Molecular Weight: 317.41
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.54 (Dichloromethane:Methanol [9:1])
HPLC: Shows >98.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.54	6.03	13.24
Found	60.72	6.02	13.19

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

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IUPAC Name: 2-[[4-(Cyclopropylcarbonyl)-1-piperazinyl]methyl]-1,2-benzisothiazol-3(2H)-one

Description:

High affinity protein disulfide isomerase (PDI) modulator ($K_d = 62$ nM). Forces PDI to adopt an oxidized conformation and suppresses its activity. Neuroprotective.

Physical and Chemical Properties:

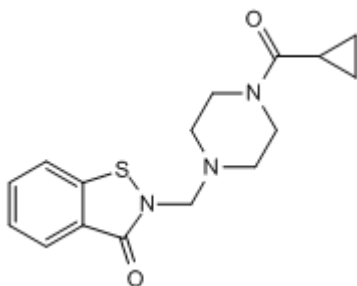
Batch Molecular Formula: $C_{16}H_{19}N_3O_2S$

Batch Molecular Weight: 317.41

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

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:

Kaplan et al (2015) Small molecule-induced oxidation of protein disulfide isomerase is neuroprotective. *Proc.Natl.Acad.Sci.U.S.A.* **112** E2245. PMID: 25848045.

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