Certificate of Analysis

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(2*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

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

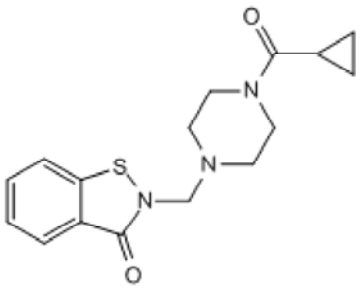
Batch Molecular Weight: 317.41

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

^{1}H 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

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Description:

LOC14 is a high affinity allosteric inhibitor of protein disulfide isomerase A3 (PDIA3) modulator (K_d = 62 nM, IC_{50} = 5 µM). In an animal model of Huntington's disease LOC14 extends survival, improves motor function, reduces ER stress from mHTT and preserves dopamine and DARPP32 levels. LOC14 is neuroprotective and rescues medium spiny neurons from neurodegeneration. LOC14 also decreases influenza A protein production in cells (IC_{50} = 4.97 µM).

Physical and Chemical Properties:

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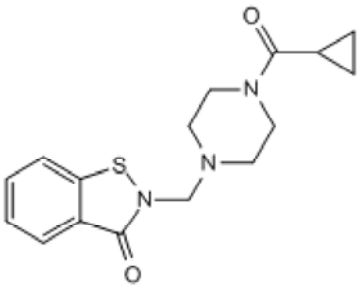
Batch Molecular Weight: 317.41

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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