

# **Certificate of Analysis**

Print Date: Oct 12th 2022

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Product Name: SSR 69071 Catalog No.: 2506 Batch No.: 2

CAS Number: 344930-95-6

IUPAC Name: 2-[[6-Methoxy-4-(1-methylethyl)-1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl]methoxy]-9-[2-(1-piperidinyl)ethoxy]-

4H-pyrido[1,2-a]pyrimidin-4-one

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{27}H_{32}N_4O_7S.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 565.64

Physical Appearance: Off-white solid

**Solubility:** ethanol to 10 mM

DMSO to 25 mM

Storage: Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.42$  (Dichloromethane:Methanol [10:1])

**HPLC:** Shows 99.4% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.33 5.88 9.91 Found 57.29 5.76 9.75

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



# **Product Information**

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#### **Description:**

SSR 69071 is a high affinity, potent inhibitor of human leukocyte elastase (HLE) (IC $_{50}$  = 3.9 nM). Displays species-selectivity ( $K_{\rm i}$  values are 0.017, 1.70, 3.01, 58 and > 100 nM for human, mouse, rat, rabbit and porcine elastase respectively). Inhibits HLE-induced lung hemorrhage in mice (ID $_{50}$  = 2.8 mg/kg) and reduces infarct size in an in vivo acute model of coronary ischemia-reperfusion injury. Orally active.

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

Batch Molecular Formula: C<sub>27</sub>H<sub>32</sub>N<sub>4</sub>O<sub>7</sub>S.½H<sub>2</sub>O

Batch Molecular Weight: 565.64 Physical Appearance: Off-white solid

**Minimum Purity:** ≥98%

#### **Batch Molecular Structure:**

**Storage:** Store at +4°C

## Solubility & Usage Info:

ethanol to 10 mM DMSO to 25 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:

**Bidouard** *et al* (2003) SSR69071, an elastase inhibitor, reduces myocardial infarct size following ischemia-reperfusion injury. Eur.J.Pharmacol. *461* 49. PMID: 12568915.

**Kapui** *et al* (2003) Biochemical and pharmacological characterization of 2-(9-(2-Piperidinoethoxy)-4-oxo-4H-pyrido[1,2- $\alpha$ ]pyrimidin-2-yloxymethyl)-4-(1-methylethyl)-6-methoxy-1,2-benzisothiazol-3(2H)-one-1,1-dioxide (SSR69071), a novel, orally active ela J.Pharmacol.Exp.Ther. *305* 451. PMID: 12606659.

Varga et al (2003) A novel orally active inhibitor of HLE. Eur.J.Med.Chem. 38 421. PMID: 12750030.

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