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Print Date: Jan 14th 2016

Certificate of Analysis

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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(3*H*)-yl]methoxy]-9-[2-(1-piperidinyl)ethoxy]-4*H*-pyrido[1,2-*a*]pyrimidin-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{32}N_4O_7S.½H_2O$

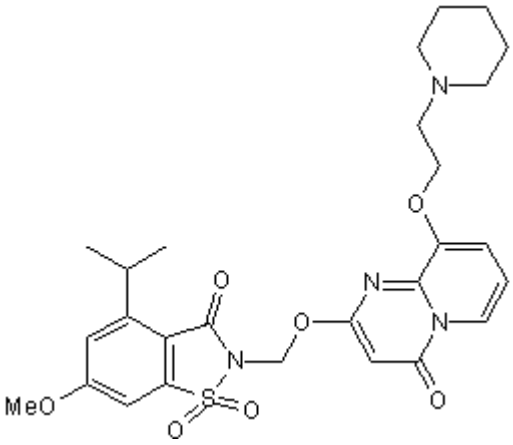
Batch Molecular Weight: 565.64

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

^{1}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

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Description:

High affinity, potent inhibitor of human leukocyte elastase (HLE) (IC_{50} = 3.9 nM). Displays species-selectivity (K_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:

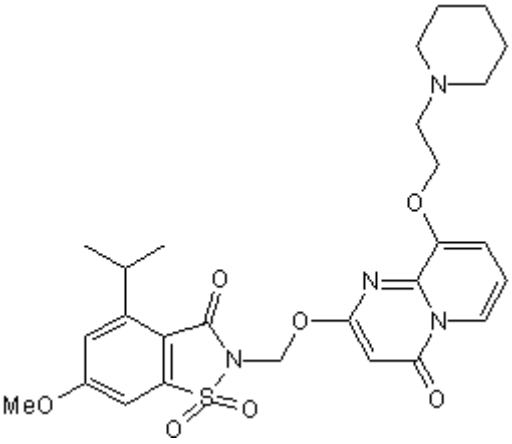
Batch Molecular Formula: $C_{27}H_{32}N_4O_7S.½H_2O$

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.

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

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

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