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Print Date: Jul 21st 2022

Certificate of Analysis

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Product Name: **SSYA10-001** **Catalog No.: 7554** **Batch No.: 1**

CAS Number: 675104-49-1

IUPAC Name: 2,4-Dihydro-5-[[(2-nitrophenyl)thio]methyl]-4-(2-propen-1-yl)-3*H*-1,2,4-triazole-3-thione

1. PHYSICAL AND CHEMICAL PROPERTIES

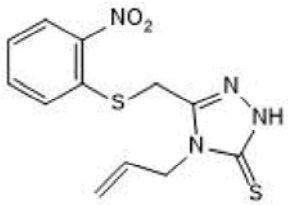
Batch Molecular Formula: $C_{12}H_{12}N_4O_2S_2$

Batch Molecular Weight: 308.37

Physical Appearance: Light green solid

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.74	3.92	18.17
Found	46.85	3.85	18.11

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Description:

SSYA10-001 is a potent coronavirus helicase inhibitor (IC_{50} values are 0.046 µM and >3 µM for unwinding and ATPase, respectively). Inhibits SARS-CoV-2 Nsp13 helicase (IC_{50} = 3.5 µM), blocks dsDNA and dsRNA unwinding activities of Nsp13 (IC_{50} values are 5.3 µM and 5.7 µM respectively). In a SARS-CoV replicon assay SSYA10-001 inhibits (+) sense but not (-) sense RNA synthesis (EC_{50} = 8.95 µM). Also inhibits human papillomavirus E6 (IC_{50} = 10 µM)

Physical and Chemical Properties:

Batch Molecular Formula: $C_{12}H_{12}N_4O_2S_2$

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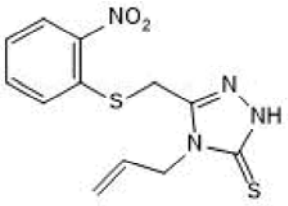
Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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:

Nizi *et al* (2022) Discovery of 2-phenylquinolines with broad-spectrum anti-coronavirus activity. ACS Med.Chem.Lett. ***13*** 855. PMID: 35571875.

Spratt *et al* (2021) Coronavirus helicases: attractive and unique targets of antiviral drug-development and therapeutic patents. Expert Opin.Ther.Pat. ***31*** 339. PMID: 33593200.

Kumar and Lupoli (2020) Exploiting existing molecular scaffolds for long-term COVID treatment. ACS Med.Chem.Lett. ***11*** 1357. PMID: 32665808.