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Certificate of Analysis

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Product Name: H10

Catalog No.: 6228 Batch No.: 1

CAS Number: IUPAC Name:

3-(N-(2-(4-((3-Carbamoylphenyl)amino)-4-oxobutanamido)ethyl)-1H-1,2,3-triazol-1-yl)ethyl)sulfamoyl)benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

2084811-68-5

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₂₄H₂₇N₇O₇S.½H₂O 566.59 White solid DMSO to 50 mM 1eq. NaOH to 20 mM Store at -20°C

Storage:

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

R _f = 0.23 (I	Dichloron	nethane	:Methanol [3:2])			
Shows 99.6% purity							
Consistent with structure							
consistent with structure							
Carbon Hydrogen Nitrogen							
Theoretical	50.88	4.98	17.3				
Found	50.77	4.91	17.18				

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

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CAS Number: IUPAC Name: 2084811-68-5

ne: 3-(*N*-(2-(4-((3-Carbamoylphenyl)amino)-4-oxobutanamido)ethyl)-1*H*-1,2,3-triazol-1-yl)ethyl)sulfamoyl)benzoic acid

Description:

H10 is a PARP14 inhibitor (IC_{50} = 490 nM). Exhibits ~ 24- and 18-fold selectivity for PARP14 over PARP1 and TNKS1, respectively. Binds both the nicotinamide and adenine sites on PARP14. Inhibits PARP14 and induces apoptosis in HepG2 and RPMI-8226 in cancer cells in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₂₇N₇O₇S.½H₂O Batch Molecular Weight: 566.59 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM 1eq. NaOH to 20 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:

Peng et al (2017) Small molecule microarray based discovery of PARP14 inhibitors. Angew.Chem.Int.Ed.Engl. 56 248. PMID: 27918638.

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