

Product Name: MS 6105

Catalog No.: 8073

Batch No.: 1

CAS Number: 2891709-58-1

IUPAC Name: 2-(5-(Cyclopropylmethyl)-3-(3-(6-(13-(((S)-1-((2S,4R)-4-hydroxy-2-((4-(4-methylthiazol-5-yl)benzyl)carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-13-oxotridecanamido)hex-1-yn-1-yl)phenyl)-4-(4-sulfamoylbenzyl)-1H-pyrazol-1-yl)thiazole-4-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₆₅H₈₁N₉O₉S₃·¼H₂O

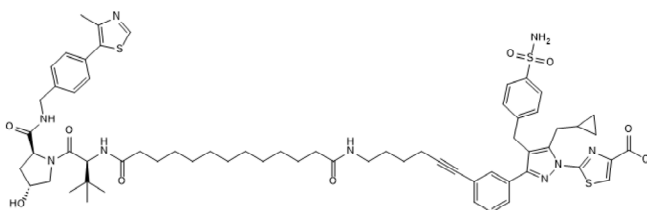
Batch Molecular Weight: 1233.1

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.31	6.66	10.22
Found	62.29	6.63	10.02

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

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Description:

MS 6105 is a potent and selective lactate dehydrogenase (LDH) Degradar (PROTAC®; for LDHA and LDHB respectively, DC₅₀ values are 38 nM and 74 nM; D_{max} is 93% and 86%). Comprises an LDH inhibitor warhead connected by a linker to a VHL ligand. Suppresses growth of several pancreatic cancer cell lines (IC₅₀ range is 12.2 μM - 16.1 μM). Bioavailable in vivo. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

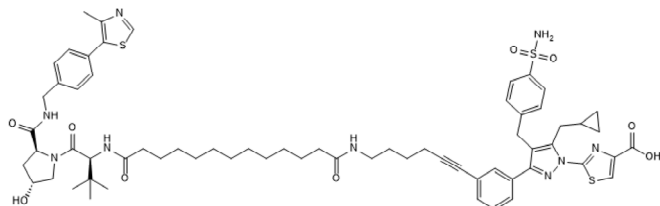
Batch Molecular Formula: C₆₅H₈₁N₉O₉S₃.¼H₂O

Batch Molecular Weight: 1233.1

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Sun *et al* (2023) Discovery of the first lactate dehydrogenase proteolysis targeting chimera degrader for the treatment of pancreatic cancer. *J.Med.Chem.* **66** 596. PMID: 36538511.

Storage: Store at -20°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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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