

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: C₆₅H₈₁N₉O₉S₃·¹/₄H₂O

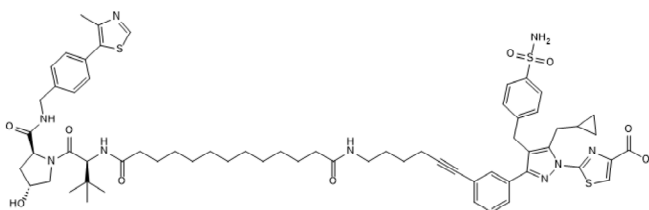
Batch Molecular Weight: 1233.1

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956

Product Name: MS 6105

Catalog No.: 8073

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

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.

Physical and Chemical Properties:

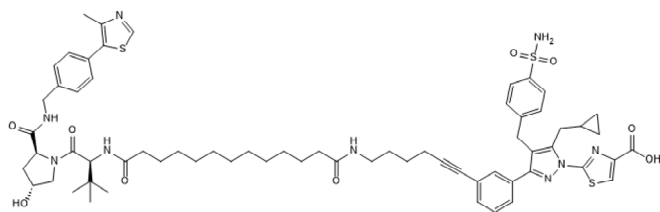
Batch Molecular Formula: C₆₅H₈₁N₉O₉S₃·¼H₂O

Batch Molecular Weight: 1233.1

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



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.

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.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956