# biotechne<sup>®</sup> TOCRIS

**IUPAC Name:** 

# **Certificate of Analysis**

## www.tocris.com

Batch No.: 1

Catalog No.: 8080

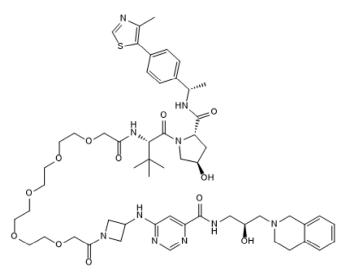
#### Product Name: MS 4322

CAS Number: 2375432-47-4

*N*-((*S*)-3-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-2-hydroxypropyl)-6-((1-((*S*)-19-((2*S*,4*R*)-4-hydroxy-2-(((*S*)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)carbamoyl)pyrrolidine-1-carbonyl)-20,20-dimethyl-17-oxo-3,6,9,12,15-pentaoxa-18-azahenicosanoyl)azetidin-3-yl)amino)pyrimidine-4-carboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C<sub>55</sub>H<sub>76</sub>N<sub>10</sub>O<sub>12</sub>S.1½H<sub>2</sub>O 1128.35 White solid DMSO to 100 mM Store at -20°C



### 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 98.2% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 58.55 7.06 12.41 Found 57.65 6.8 11.95

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

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# Print Date: Dec 13th 2024

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*N*-((*S*)-3-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-2-hydroxypropyl)-6-((1-((*S*)-19-((2*S*,4*R*)-4-hydroxy-2-(((*S*)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)carbamoyl)pyrrolidine-1-carbonyl)-20,20-dimethyl-17-oxo-3,6,9,12,15-pentaoxa-18-azahenicosanoyl)azetidin-3-yl)amino)pyrimidine-4-carboxamide

#### **Description:**

MS 4322 is a protein arginine methyltransferase 5 (PRMT5) Degrader (PROTAC®) (DC<sub>50</sub> = 1.1  $\mu$ M, D<sub>max</sub> = 74% in MCF-7 cells). Inhibits PRMT5 methyltransferase activity (IC<sub>50</sub> = 18 nM) and dose-dependently inhibits proliferation of HeLa, A549, A172 and Jurkat cancer cell lines. Comprises a PRMT5 inhibitor linked to an E3 ligase ligand.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>55</sub>H<sub>76</sub>N<sub>10</sub>O<sub>12</sub>S.1½H<sub>2</sub>O Batch Molecular Weight: 1128.35 Physical Appearance: White solid

### Minimum Purity: ≥98%

#### **Batch Molecular Structure:**

#### **Storage:** Store at -20°C

Solubility & Usage Info: DMSO to 100 mM

#### Stability and Solubility Advice:

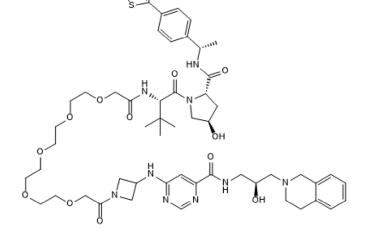
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Catalog No.: 8080

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:

Shen et al (2020) Discovery of first-in-class protein arginine methyltransferase 5 (PRMT5) degraders. J.Med.Chem. 63 9977. PMID: 32787082.

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