

**Product Name:** cis-SIM1

**Catalog No.:** 7433

**Batch No.:** 1

CAS Number: 2719051-98-4

IUPAC Name: *N,N'*-(11-((2-(((S)-1-((2*S*,4*S*)-4-Hydroxy-2-((4-(4-methylthiazol-5-yl)benzyl)carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-2-oxoethoxy)methyl)-11-methyl-3,6,9,13,16,19-hexaoxahenicosane-1,21-diyl)bis(2-((S)-4-(4-chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)acetamide)

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>79</sub>H<sub>98</sub>Cl<sub>2</sub>N<sub>14</sub>O<sub>13</sub>S<sub>3</sub>·3½H<sub>2</sub>O

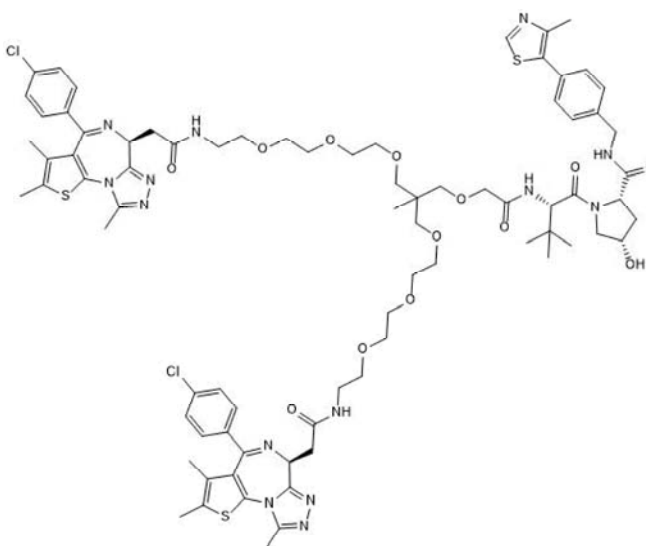
**Batch Molecular Weight:** 1681.87

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	56.42	6.29	11.66
Found	55.99	5.86	11.51

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**Product Name:** cis-SIM1

**Catalog No.:** 7433

**1**

CAS Number: 2719051-98-4

IUPAC Name: *N,N'*-(11-((2-(((S)-1-((2*S*,4*S*)-4-Hydroxy-2-((4-(4-methylthiazol-5-yl)benzyl)carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-2-oxoethoxy)methyl)-11-methyl-3,6,9,13,16,19-hexaoxahenicosane-1,21-diyl)bis(2-((S)-4-(4-chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)acetamide)

**Description:**

cis-SIM1 is the negative control for SIM1 (Cat. No. 7432).

**Physical and Chemical Properties:**

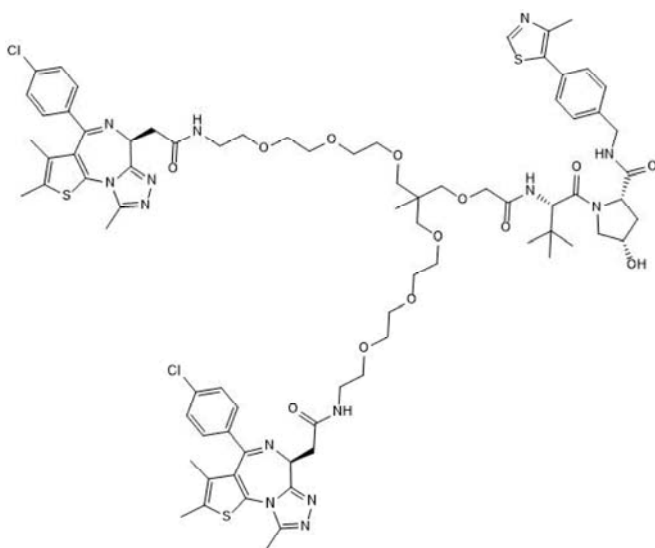
Batch Molecular Formula: C<sub>79</sub>H<sub>98</sub>Cl<sub>2</sub>N<sub>14</sub>O<sub>13</sub>S<sub>3</sub>·3½H<sub>2</sub>O

Batch Molecular Weight: 1681.87

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).

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.

**Licensing Information:**

Sold under licence from the University of Dundee

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