

Product Name: CST 626

Catalog No.: 8021

Batch No.: 1

CAS Number: 3033993-13-1

IUPAC Name: (2*S*,4*S*)-1-((*S*)-2-Cyclohexyl-2-((*S*)-2-(methylamino)propanamido)acetyl)-4-(3-((5-(((*S*)-1-((2*S*,4*R*)-4-hydroxy-2-(((*S*)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-5-oxopentyl)oxy)phenoxy)-*N*-((*R*)-1,2,3,4-tetrahydronaphthalen-1-yl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₆₁H₈₂N₈O₉S·¾H₂O

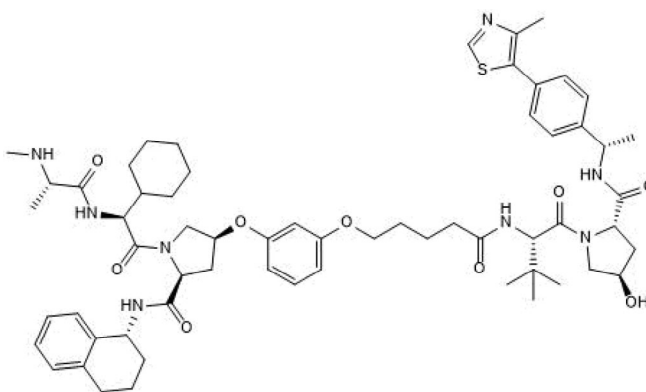
Batch Molecular Weight: 1116.94

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 65.6 | 7.54 | 10.03 |
| Found | 64.55 | 7.46 | 9.72 |

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

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Description:

CST 626 is a potent IAP Degradator (PROTAC®) (DC₅₀ values at 16 hours are 0.7 nM, 2.4 nM and 6.2 nM at XIAP, cIAP1 and cIAP2 respectively; D_{max} = 90-99%). Reduces cell viability in some cell types, including SUDHL6 and MOLM13 (IC₅₀ values are 16 nM and 21 nM respectively). PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

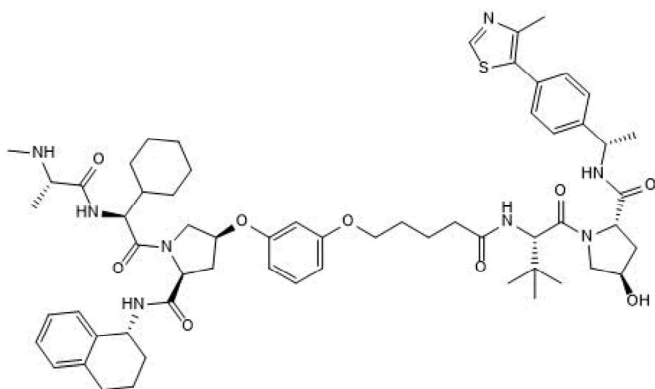
Batch Molecular Formula: C₆₁H₈₂N₈O₉S.¾H₂O

Batch Molecular Weight: 1116.94

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Ng *et al* (2023) Heterobifunctional ligase recruiters enable pan-degradation of inhibitor of apoptosis proteins. *J.Med.Chem.* **66** 4703. PMID: 36996313.

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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