(S,R,S)-AHPC-C6-PEG3-C4-Cl

Cat. No.: HY-103605

CAS No.: 1835705-55-9

Molecular Formula: $C_{38}H_{59}ClN_4O_7S$

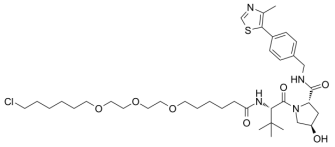
Molecular Weight: 751.42

Target: E3 Ligase Ligand-Linker Conjugates

Pathway: PROTAC

Storage:

Pure form	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (133.08 mM)

Ethanol : 100 mg/mL (133.08 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.3308 mL	6.6541 mL	13.3081 mL
5 mM	0.2662 mL	1.3308 mL	2.6616 mL
10 mM	0.1331 mL	0.6654 mL	1.3308 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (3.33 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (3.33 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(S,R,S)-AHPC-C6-PEG3-C4-Cl (VH032-C6-PEG3-C4-Cl) is a conjugate of ligands for E3 and 20-atom-length linker. The connector of linker is Halogen group. (S,R,S)-AHPC-C6-PEG3-C4-Cl incorporates the (S,R,S)-AHPC based VHL ligand and an alkyl/ether-based linker. (S,R,S)-AHPC-C6-PEG3-C4-Cl is capable of inducing the degradation of GFP-HaloTag7 in cell-based assays[1].

IC_{50} & Target

VHL

In Vitro

(S,R,S)-AHPC-C6-PEG3-C4-Cl uses the cereblon ligand[1]. The linker is 6-2-2-6. The linkers contain a mixture of hydrophobic

and hydrophilic moieties to balance the hydrophobicity/hydrophilicity of the resulting hybrid compounds. PROTACs that induce the degradation of an oncogenic tyrosine kinase, BCR-ABL has been developed. (S,R,S)-AHPC-C6-PEG3-C4-Cl can be attached to potent TKIs (bosutinib and dasatinib) that mediate the degradation of c-ABL and BCR-ABL by hijacking either CRBN or VHL E3 ubiquitin ligase [2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. US 20170121321 A1

[2]. Lai AC, et al. Modular PROTAC Design for the Degradation of Oncogenic BCR-ABL. Angew Chem Int Ed Engl. 2016 Jan 11;55(2):807-10.

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