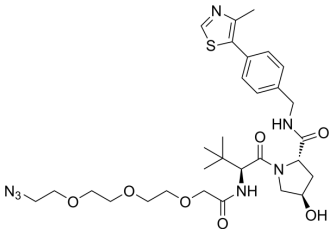
(S,R,S)-AHPC-PEG3-N3

Cat. No.:	HY-103598
CAS No.:	1797406-80-4
Molecular Formula:	$C_{30}H_{43}N_7O_7S$
Molecular Weight:	645.77
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

Ethanol : 100 mg/mL (154.85 mM; Need ultrasonic)

H_2O : ≥ 100 mg/mL (154.85 mM)

DMSO : 50 mg/mL (77.43 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5485 mL	7.7427 mL	15.4854 mL
	5 mM	0.3097 mL	1.5485 mL	3.0971 mL
	10 mM	0.1549 mL	0.7743 mL	1.5485 mL

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

BIOLOGICAL ACTIVITY

Description

(S,R,S)-AHPC-PEG3-N3 is a synthesized E3 ligase ligand-linker conjugate that incorporates the (S,R,S)-AHPC based VHL ligand and 3-unit PEG linker used in PROTAC technology. (S,R,S)-AHPC-PEG3-N3 is a click chemistry reagent, it contains an Azide group and can undergo copper-catalyzed azide-alkyne cycloaddition reaction (CuAAc) with molecules containing Alkyne groups. Strain-promoted alkyne-azide cycloaddition (SPAAC) can also occur with molecules containing DBCO or BCN groups.

IC_{50} & Target

VHL

In Vitro

(S,R,S)-AHPC-PEG3-N3 is extracted from patent WO/2016/146985A1, figure 11. PROTAC has been developed having structure A-L-B that can tether a bromodomain inhibitor via a moiety which binds to a protein within the bromo- and Extra-terminal (BET) family of proteins to a small molecule E3 ubiquintin ligase protein binding ligand compond via a suitable linker[1][2].

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

REFERENCES

[1]. CIULLI, Alessio, et al. DERIVATIVES OF 1-[(CYCLOPENTYL OR 2-PYRROLIDINYL)CARBONYLAMINOMETHYL]-4-(1,3-THIAZOL-5-YL) BENZENE WHICH ARE USEFUL FOR THE TREATMENT OF PROLIFERATIVE, AUTOIMMUNE OR INFLAMMATORY DISEASES. WO2016146985A1.

[2]. Zengerle M, et al. Selective Small Molecule Induced Degradation of the BET Bromodomain Protein BRD4. ACS Chem Biol. 2015 Aug 21;10(8):1770-7.

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