MedChemExpress
(S,R,S)-AHPC-PEG2-C4-Cl

| Cat. No.: | $\mathrm{HY}-103607$ |  |
| :--- | :--- | :--- |
| CAS No.: | $1835705-57-1$ |  |
| Molecular Formula: | $\mathrm{C}_{32} \mathrm{H}_{47} \mathrm{ClN}_{4} \mathrm{O}_{6} \mathrm{~S}$ |  |
| Molecular Weight: | 651.26 |  |
| Target: | E3 Ligase Ligand-Linker Conjugates |  |
| Pathway: | PROTAC |  |
| Storage: | Pure form | $-20^{\circ} \mathrm{C}$ |
|  |  | $4^{\circ} \mathrm{C}$ |
|  |  | 3 years |
|  | In solvent | $-80^{\circ} \mathrm{C}$ |
|  |  | $-20^{\circ} \mathrm{C}$ |
|  |  | 1 months |



## SOLVENT \& SOLUBILITY

## In Vitro

DMSO : $\geq 50 \mathrm{mg} / \mathrm{mL}(76.77 \mathrm{mM})$
$\mathrm{H}_{2} \mathrm{O}: 50 \mathrm{mg} / \mathrm{mL}(76.77 \mathrm{mM}$; Need ultrasonic)
Ethanol : $50 \mathrm{mg} / \mathrm{mL}(76.77 \mathrm{mM}$; Need ultrasonic)

* " $^{2} \geq$ " means soluble, but saturation unknown.

|  | Solvent Mass |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
| Concentration | 1 mg | 5 mg | 10 mg |  |
| Preparing <br> Stock Solutions | 1 mM |  |  |  |
|  | 5 mM | 1.5355 mL | 7.6774 mL | 15.3548 mL |

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

## BIOLOGICAL ACTIVITY

Description
$\mathrm{IC}_{50}$ \& Target VHL

In Vitro
(S,R,S)-AHPC-PEG2-C4-Cl (VH032-PEG2-C4-Cl) is a conjugate of ligands for E3 and 13-atom-length linker. The connector of linker is Halogen group. (S,R,S)-AHPC-PEG2-C4-Cl incorporates the (S,R,S)-AHPC based VHL ligand and an alkyl/ether-based linker. (S,R,S)-AHPC-PEG2-C4-Cl is capable of inducing the degradation of GFP-HaloTag7 in cell-based assays ${ }^{[1]}$.
(S,R,S)-AHPC-PEG2-C4-Cl uses the VHL ligand ${ }^{[1]}$. 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-PEG2-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]. Craig Crews, et al. Proteolysis Targeting Chimera Compounds and Methods of Preparing and Using Same. US20170121321A1.
[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.

## Caution: Product has not been fully validated for medical applications. For research use only.

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