AT6

Cat. No.: HY-112375

CAS No.: 2098836-50-9

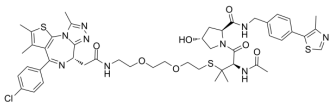
Molecular Formula: $C_{48}H_{58}ClN_9O_7S_3$

Molecular Weight: 1004.68

Target: PROTACs

Pathway: PROTAC

Storage: -20°C, protect from light, stored under nitrogen
* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (99.53 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	0.9953 mL	4.9767 mL	9.9534 mL
	5 mM	0.1991 mL	0.9953 mL	1.9907 mL
	10 mM	0.0995 mL	0.4977 mL	0.9953 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: ≥ 5 mg/mL (4.98 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (4.98 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (4.98 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

AT6 is a PROTAC AT1 analogue, which is a PROTAC connected by ligands for von Hippel-Lindau and BRD4 with highly selectivity to bromodomain (Brd4).

In Vitro

PROTACs (proteolysis-targeting chimaeras) are bifunctional molecules that recruit a target protein in proximity to an E3 ubiquitin ligase to trigger protein degradation. Structural elucidation of the key ternary ligase: PROTAC: target species and how this impacts target degradation selectivity remains elusive. The ligand folds into itself to allow formation of specific intermolecular interactions in the ternary complex. Isothermal titration calorimetry studies, supported by surface mutagenesis and proximity assays, are consistent with pronounced cooperative formation of ternary complexes with Brd4

	^{BD2}. Structure-based-designed compound AT1 exhibits highly selective depletion of Brd4 in cells[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Gadd MS, et al. Structural basis of PROTAC cooperative recognition for selective protein degradation. Nat Chem Biol. 2017 May;13(5):514-521.

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