

Product Data Sheet

Product Name: AT6
Cat. No.: GC33354

Chemical Properties

Cas. No. 2098836-50-9

SMILES CC1=C(C)C(C(C2=CC=C(Cl)C=C2)=N[C@@H](CC(NCCOCCOCCSC(C)(C)[C@H](NC(C)=O)C(N3C[C@H](O)C[C@H]3C(NCC4=CC=C(C5=C(C)N=CS5)C=C4)=O)=O)C6=NN=C(C)N67)=C7S1

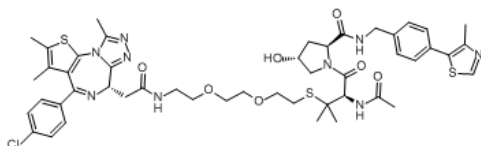
Formula C₄₈H₅₈ClN₉O₇S₃ M.Wt 1004.68

Solubility Soluble in DMSO Storage Store at -20°C, protect from light, stored under nitrogen

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

AT6 is a PROTAC AT1 analogue, which is a highly selective bromodomain (Brd4) degrader.

PROTACs (proteolysis-targeting chimerae) are bifunctional molecules that recruit a target protein in proximity to an E3 ubiquitin ligase to trigger protein degradation. Structural elucidation of the key

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

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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 Brd4BD2. Structure-based-designed compound AT1 exhibits highly selective depletion of Brd4 in cells[1].

[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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