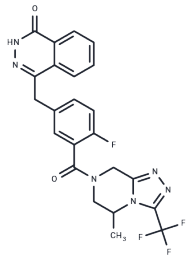
Data Sheet (Cat.No.T63228)

TargetMol

Simmiparib

Chemical Properties



CAS No. : 1551355-46-4

Formula: C23H18F4N6O2

Molecular Weight: 486.42

Storage: Store at low temperature,Keep away from direct sunlight,Keep away from moisture
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Simmiparib (SMOCL-9112) is a novel and potent PARP1 and PARP2 inhibitor, a derivative of Olaparib.Simmiparib induces DNA double-strand breaks (DSBs) and cell cycle arrest in homologous recombination repair (HR)-deficient cells, thereby contributing to apoptosis.Simmiparib has been used for study Parkinson's disease, Alzheimer's disease, breast cancer, and melanoma.
Targets(IC50)	Apoptosis,PARP
In vitro	Simmiparib, when applied at concentrations ranging from 0 to 10 μM for 3 days, demonstrates anti-proliferative activity against various cancer cells[1]. In Capan-1 cells, Simmiparib induces typical G2/M arrest when administered at concentrations of 0-10 μM for 48 hours[1]. Apoptosis is induced in MDA-MB-436 and V-C8 (BRCA2-/-) cells by Simmiparib at concentrations of 0.1-2 μM for 24 hours. Additionally, there is a dose-dependent increase in the levels of γH2AX[1].Furthermore, treatment with Simmiparib at concentrations of 1-10 μM for 48 or 72 hours increases the phosphorylation levels of Chk1 and Chk2. Additionally, it enhances the protein levels of p-Cyclin B1 (S147), Cyclin B1, p-CDK1 (Y15), and CDK1[1].
In vivo	In xenograft mouse models, Simmiparib inhibits the growth of tumors in V-C8 (BRCA2-/-) and MDA-MB-436 (BRCA2-/-) when administered orally at doses of 2, 4, and 8 mg/kg once daily for 14 days[1].Additionally, Simmiparib, at doses of 10 and 50 mg/kg administered orally once daily for 42 days, inhibits the growth of BRCA1-mutated breast cancer in xenograft mouse models[1].

Solubility Information

Solubility	DMSO: 80 mg/mL (164.47 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0558 mL	10.2792 mL	20.5584 mL
5 mM	0.4112 mL	2.0558 mL	4.1117 mL
10 mM	0.2056 mL	1.0279 mL	2.0558 mL
50 mM	0.0411 mL	0.2056 mL	0.4112 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Yuan B, et al. Poly(ADP-ribose)polymerase (PARP) inhibition and anticancer activity of simmiparib, a new inhibitor undergoing clinical trials. Cancer Lett. 2017 Feb 1;386:47-56.