Data Sheet (Cat.No.T61530)

TargetMol

PBENZ-DBRMD

Chemical Properties

CAS No. : 1454662-41-9

Formula: C11H5Br2NO4

Molecular Weight: 374.97

Storage: 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	PBENZ-DBRMD (4-(3,4-Dibromo-2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)benzoic acid) is a potent inhibitor of type 3 iodothyronine deiodinase (DIO3). It not only suppresses cell proliferation but also induces apoptosis, holding potential value for cancer research.
Targets(IC50)	Apoptosis
In vitro	Method: DIO3-positive HGSOC cells (OVCAR3 and KURAMOCHI) and DIO3-negative normal ovary cells (CHOK1) were treated with PBENZ-DBRMD (0.5, 1, 10 μM) for 96 h, with daily administration. Cell density was observed using light microscopy. Cell counting was performed by flow cytometry. Apoptosis was assessed by Annexin-PI staining, cell cycle analysis was conducted, cell proliferation was measured using the CyQUANT assay, and DIO3 as well as proliferation-related protein expression were detected by Western blot. Result: PBENZ-DBRMD dose-dependently reduced the number of DIO3-positive HGSOC cells, induced apoptosis (increased percentages of Annexin+/PI- and Annexin+/PI+ cells), increased the proportion of cells in the Sub-G1 phase, and significantly inhibited cell proliferation, while having no obvious effect on DIO3-negative CHOK1 cells. Under DIO3 knockdown or T3-deficient conditions, PBENZ-DBRMD lost its antitumor efficacy. Western blot analysis showed that PBENZ-DBRMD reduced the expression of the DIO3 dimer (75 kDa) and downregulated various pro-cancer proteins, including mutant p53, PKM2, c-Myc, pERK, PCNA, Cyclin D1, and CDK4 [1].
In vivo	Method: OVCAR3 cells were subcutaneously injected into the left flank of female nude mice to establish an HGSOC xenograft model. Eleven days after tumor inoculation, mice were randomly divided into three groups (n = 6) and treated with daily intraperitoneal injections of PBENZ-DBRMD (5 mM, approximately 18.5 mg/kg), ITYR-DBRMD, or vehicle control (5% DMSO-PBS), five days per week for three weeks. Tumor volume and weight were measured. Western blot analysis was performed to detect the expression of relevant proteins in tumor tissues. IHC was used to detect DIO3 and Ki67 expression, and H&E staining was conducted to observe tissue morphology. Result: PBENZ-DBRMD significantly inhibited tumor volume growth and reduced tumor weight (p = 0.054, borderline significant). The expression of β-catenin, PAX8, mutant p53, PCNA, Cyclin D1, and CDK4 was decreased in tumor tissues. IHC showed a marked reduction in the positive rates of membranous DIO3 and Ki67 in tumor tissues. In the DIO3-knockdown OVCAR3 cell transplantation model, PBENZ-DBRMD had no significant effect on tumor volume or weight, further confirming that its antitumor effect is

In vivo	dependent on DIO3 expression [1].

Solubility Information

Solubility	DMSO: 80 mg/mL (213.35 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6669 mL	13.3344 mL	26.6688 mL
5 mM	0.5334 mL	2.6669 mL	5.3338 mL
10 mM	0.2667 mL	1.3334 mL	2.6669 mL
50 mM	0.0533 mL	0.2667 mL	0.5334 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

Moskovich D, et al. Targeting the DIO3 enzyme using first-in-class inhibitors effectively suppresses tumor growth: a new paradigm in ovarian cancer treatment. Oncogene. 2021;40(44):6248-6257.