Product Data Sheet

Product Name: BRCA1-IN-1
Cat. No.: GC33223

Chemical Properties

Cas. No.	1622262-74-1		
SMILES	O=C(N[C@@H](CC(F)(F)P(O)(O)=O)C(NCC(NCCCCC1=CC=CC=C1)=O)=O)CCC2=CNC3=C2C=CC=C3		
Formula	$C_{27}H_{33}F_2N_4O_6P$	M.Wt	578.54
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	BRCA1-IN-1		

Background

BRCA1-IN-1 is a novel small-molecule-like BRCA1 inhibitor with IC50 and Ki of 0.53 μM and 0.71 μM, respecrively.

BRCTs are phosphoserine-binding domains found in proteins involved in DNA repair, DNA damage response and cell cycle regulation. BRCA1 is a BRCT domain-containing, tumor-suppressing protein expressed in the cells of breast and other tissues. By targeting the (BRCT)2 domain, BRCA1-IN-1 (Compound 15a) inhibits BRCA1 activities in tumor cells, sensitizes these cells to ionizing radiation-induced apoptosis, and shows synergistic inhibitory effect when used in combination with Olaparib (a small-molecule inhibitor of poly-ADP-ribose polymerase) and Etoposide (a small-molecule inhibitor of topoisomerase II). BRCA1-IN-1 can effectively inhibit HR activity by binding to BRCA1(BRCT)2, and functionally mimic genetic knockdown of BRCA1. BRCA1-IN-1 is useful in targeting BRCA1/PARP-related pathways involved in DNA damage and repair response, for cancer therapy. The synergistic inhibition of PARP/BRCA1 (a process referred to as synthetic lethality), is highly effective in cancer therapy. BRCA1-IN-1 is small-molecule-like and can be directly administered to tumor cells, thus making them useful for future studies

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of BRCA1/PARP-related pathways in DNA damage and repair response, and in cancer therapy[1].

[1]. Na Z, et al. Discovery of cell-permeable inhibitors that target the BRCT domain of BRCA1 protein by using a small-molecule microarray. Angew Chem Int Ed Engl. 2014 Aug 4;53(32):8421-6.

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