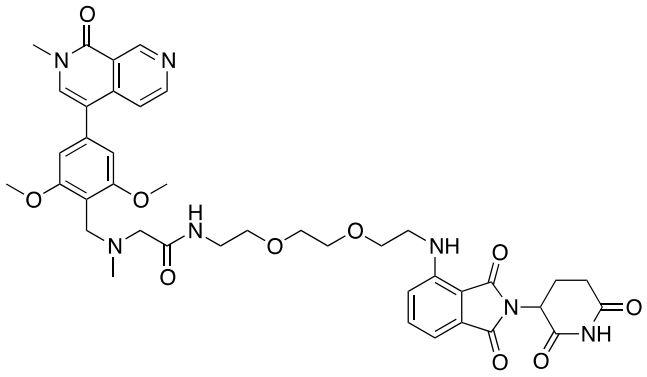
dBRD9



Chemical Formula: $C_{40}H_{45}N_7O_{10}$
Molecular Weight: 783.83

Category	Parameter	Description
Compound	Name	dBRD9
	Citation	*Angewandte Chemie* **2017**, *56(21),* 5738-5743
	Chemical descriptors	O=C1C2=C(C=CN=C2)C(C3=CC(OC)=C(CN(C)CC(NCCOCCOCCNC4=C5C(C(N(C6C(NC(CC6)=O)=O)C5=O)=O)=CC=C4)=O)C(OC)=C3)=CN1C
	Chemical name	2-((2,6-dimethoxy-4-(2-methyl-1-oxo-1,2-dihydro-2,7-naphthyridin-4-yl)benzyl)(methyl)amino)-*N*-(2-(2-(2-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)amino)ethoxy)ethoxy)ethyl)acetamide
	Entries in chemical databases	**CID** N/A
	Availability	Gray Lab
In vitro profiling	Target (potency)	BRD9 (104 nM IC50 (AlphaScreen), 100% Inhibition @ 1 uM (BromoScan))
	Target (potency)	BRD9 (> 90% degradation (4 hrs 100 nM, MOLM-13, EOL-1 Cell lines))
	Selectivity	Off-target degradation of IKZF family observed in select lymphoid tissues
	Potential reactivity	Unstable to basic hydrolysis
	SAR	See: Supplemental Information; *Angewandte Chemie* **2017**, *56(21),* 5738-5743
	Mechanism of inhibition	Bi-functional targeted degradation
	Structure of target-probe complex	5TWX
Cellular profiling	Validation of cellular target	Domain swap BRD9 resistance alleles rescue cytostasis in MOLM-13 AML.
	Validation of cellular specificity	Global proteomic degradation profiling at 2hrs.
Pharmacodynamics		dBRD9 significantly inhibited tumor progression in a murine model of synovial sarcoma.
Pharmacokinetics		N/A

Synthetic scheme