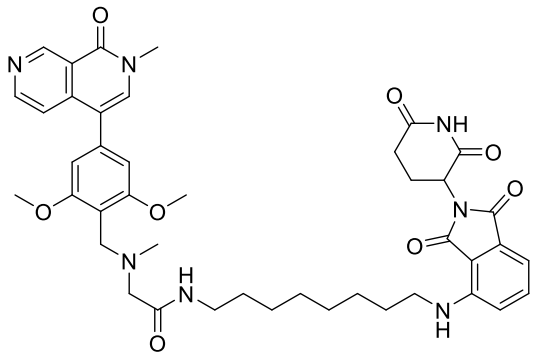
dBRD9-A



Chemical Formula: $C_{42}H_{49}N_7O_8$
Molecular Weight: 779.8950

Category	Parameter	Description
Compound	Name	dBRD9-A
	Citation	eLife 2018;7:e41305. DOI: https://doi.org/10.7554/eLife.41305
	Chemical descriptors	O=C1N(C(CCC(N2)=O)C2=O)C(C3=C(NCCCCCCCCNC(CN(C)CC(C(OC)=C4)=C(OC)C=C4C5=CN(C)C(C6=C5C=CN=C6)=O)=O)C=CC=C31)=O
	Chemical name	2-((2,6-dimethoxy-4-(2-methyl-1-oxo-1,2-dihydro-2,7-naphthyridin-4-yl)benzyl)(methyl)amino)-N-(8-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)amino)octyl)acetamide
	Entries in chemical databases	
	Availability	Gray Lab
In vitro profiling	Target (potency)	BRD9 (83.1 nM IC50 (AlphaScreen)
	Target (potency)	BRD9 (> 90% degradation (6 hrs 100 nM, HSSY1, SYO1))
	Selectivity	Off-target degradation of IKZF family observed in select lymphoid tissues
	Potential reactivity	Unstable to basic hydrolysis
	SAR	See: *Angewandte Chemie International Edition* 56.21 (2017): 5738-5743. DOI: https://doi.org/10.1002/anie.201611281
	Mechanism of inhibition	Bi-functional targeted degradation
	Structure of target-probe complex	N/A
Cellular profiling	Validation of cellular target	Domain swap BRD9 resistance alleles rescue cytostasis in synovial sarcoma.
	Validation of cellular specificity	N/A
Pharmacodynamics		dBRD9-A significantly inhibited tumor progression in a murine model of synovial sarcoma.
Pharmacokinetics		N/A

Synthetic scheme