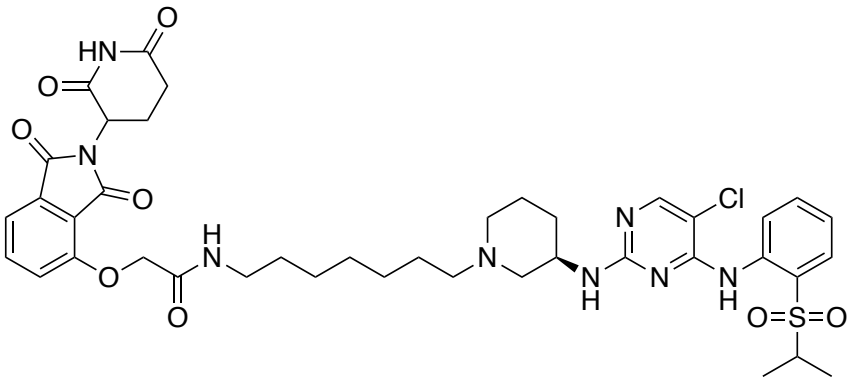
BSJ-4-116



Chemical Formula: $C_{40}H_{49}ClN_8O_8S$
Exact Mass: 836.31
Molecular Weight: 837.39

Category	Parameter	Description
Compound	Name	BSJ-4-116
	Citation	Nat Chem Biol 2021, 17, 675–683
	Chemical descriptors	CC(S(=O)(C1=CC=CC=C1NC2=NC(N[C@@H]3CCCN(C3)CCCCCCCNC(COC4=CC=CC5=C4C(N(C5=O)C6CCC(NC6=O)=O)=O)=O)=NC=C2Cl)=O)C
	Chemical name	N-(7-((R)-3-((5-chloro-4-((2-(isopropylsulfonyl)phenyl)amino)pyrimidin-2-yl)amino)piperidin-1-yl)heptyl)-2-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)oxy)acetamide
	Entries in chemical databases	CID 155235839
	Availability	Medchem Express https://www.medchemexpress.com/bsj-4-116.html
In vitro profiling	Target (potency)	CDK12/Cyc K 6nM
	Target (potency)	
	Selectivity	Kinomescan S(10)=0.017, profiled at a concentration of 1 μM against a panel of 468 human kinases
	Potential reactivity	
	SAR	
	Mechanism of inhibition	Protein degradation by recruiting Cereblon
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	BSJ-4-116 exhibited potent CDK12 degradation in Jurkat cells in a dose- and time-dependent manner, whereas CDK13 protein level was minimally affected
	Validation of cellular specificity	The selectivity for CDK12 degradation was assessed by proteome-wide profiling using Jurkat cells that were treated with 50 nM BSJ-4-116 for 8 h
Pharmacodynamics		
Pharmacokinetics		

Synthetic scheme