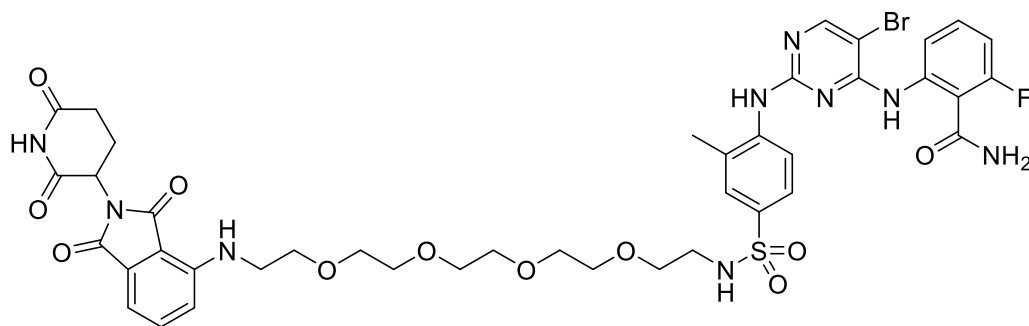


TMX-2172



Chemical Formula: C₄₁H₄₅BrFN₉O₁₁S
Molecular Weight: 970.83

Category	Parameter	Description
Compound	Name	TMX-2172
	Citation	Angew. Chem. Int. Ed., 2020, 59, 13865-13870 https://doi.org/10.1002/anie.202004087
	Chemical descriptors	BrC1=CN=C(NC2=C(C)C=C(S(NCCOCCOCCOCCOCCOCCNC3=C(C(N(C4CCC(NC4=O)=O)C5=O)=O)C5=CC=C3)(=O)=O)C=C2)N=C1NC6=C(C(N)=O)C(F)=CC=C6
	Chemical name	2-((5-bromo-2-((4-(N-(14-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisindolin-4-yl)amino)-3,6,9,12-tetraoxatetradecyl)sulfamoyl)-2-methylphenyl)amino)pyrimidin-4-yl)amino)-6-fluorobenzamide
	Entries in chemical databases	N/A
	Availability	N/A
	Additional comments	Negative control ZXH-7035 is also available
<i>In vitro</i> profiling	Target (potency)	CDK2: 6.5 nM (ZYLTE); CDK5: 6.8 nM (ZYLTE); CDK1: 20.3 nM (ZYLTE)
	Selectivity	KiNativ at 1 μM (LRRK2, JNK1/2/3, CDK2, CDK5, AURKA)
	Potential reactivity	Lenalidomide motif
	SAR	N/A
	Mechanism of inhibition	Proteasome degradation
	Structure of target-probe complex	N/A
	Additional comments	N/A
Cellular profiling	Validation of cellular target	Target degradation and rescue
	Validation of cellular specificity	Proteomics in OVCAR8
	Additional comments	
Pharmacodynamics		N/A
Pharmacokinetics		N/A

Synthetic scheme

