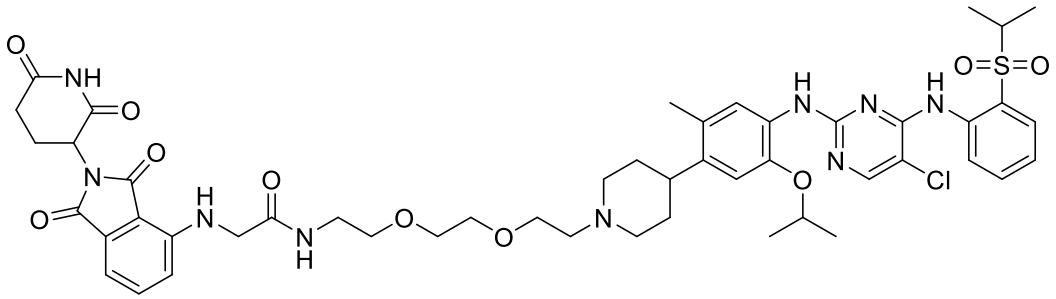
TL13-112



Chemical Formula: $C_{49}H_{60}ClN_9O_{10}S$
Molecular Weight: 1002.5820

Category	Parameter	Description
Compound	Name	TL13-112
	Citation	*J. Med. Chem.* **2018**, 61, 9, 4249-4255 https://pubs.acs.org/doi/10.1021/acs.jmedchem.7b01655
	Chemical descriptors	CC(C)OC1=CC(C2CCN(CCOCCOCCNC(=O)CNC3=CC=CC4=C3C(=O)N(C3CCC(=O)NC3=O)C4=O)CC2)=C(C)C=C1NC1=NC=C(Cl)C(NC2=CC=CC=C2S(=O)(=O)C(C)C)=N1
	Chemical name	N-(2-(2-(2-(4-(4-((5-Chloro-4-((2-(isopropylsulfonyl)phenyl)- amino)pyrimidin-2-yl)amino)-5-isopropoxy-2-methylphenyl)- piperidin-1-yl)ethoxy)ethoxy)ethyl)-2-((2-(2,6-dioxopiperidin- 3-yl)-1,3-dioxoisoindolin-4-yl)amino)acetamide
	Entries in chemical databases	**CID:** 138108958
	Availability	
In vitro profiling	Target (potency)	ALK (IC_{50} 26.4 nM in H3122 cellular assay, IC_{50} 0.6 nM in biochemical activity assay)
	Target (potency)	FAK (IC_{50} 25.4 nM in Z'LYTE assay), FER (IC_{50} 42.4 nM in Z'LYTE assay), RSK1 (IC_{50} 677 nM in Z'LYTE assay), Aurora A (IC_{50} 8550 nM in Z'LYTE assay)
	Selectivity	
	Potential reactivity	
	SAR	
	Mechanism of inhibition	Reversible small molecule degrader
	Structure of target-probe complex	
	Additional comments	CRBN engaging degrader. Negative control TL13-110 is also available
Cellular profiling	Validation of cellular target	TL13-112 dose dependently inhibited the growth of the ALK-positive cell lines H3122, Karpas 299, SU-DHL-1, Kelly, Lan5, SH-SY5Y, and CHLA20
	Validation of cellular specificity	
Pharmacodynamics		TL13-112 inhibited ALK phosphorylation and downstream STAT3 phosphorylation in H3122, Karpas 299, Kelly, and CHLA20 cells
Pharmacokinetics		

Synthetic scheme