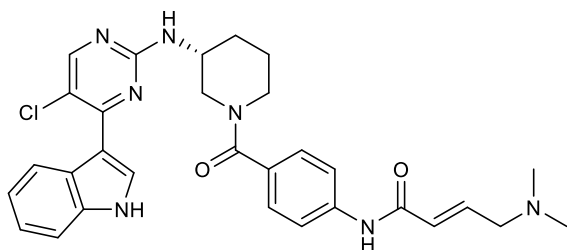


THZ531



Chemical Formula: $C_{30}H_{32}ClN_7O_2$

Exact Mass: 557.231

Category	Parameter	Description
Compound	Name	THZ531
	Citation	Nat Chem Biol. 2016; 12(10): 876–884
	Chemical descriptors	<chem>C1C=CN=C(N[C@H]2CN(C(C3=CC=C(NC(/C=C/CN(C)C)=O)C=C3)=O)CCC2)N=C1C4=CNC5=C4C=CC=C5</chem>
	Chemical name	(R,E)-N-(4-(3-((5-chloro-4-(1H-indol-3-yl)pyrimidin-2-yl)amino)piperidine-1-carbonyl)phenyl)-4-(dimethylamino)but-2-enamide
	Entries in chemical databases	
<i>In vitro</i> profiling	Availability	APEXBio https://www.apexbt.com/thz531.html?gclid=EAlaIqobChMImqbOsqv41wVII2zCh3wNgmWEAAAYASAAEgJ13vD_BwE
	Target (potency)	CDK12 (IC ₅₀ 158 biochemical assay) CDK13 ((IC ₅₀ 69 nM biochemical assay)
	Selectivity	Good
	Potential reactivity	Cyteine reactive
	SAR	
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	5ACB
Cellular profiling	Validation of cellular target	CTD-phosphorylation and competition pulldown with THZ1-biotin
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		T _{1/2} 0.49h, AUC 276 (ng*hr/mL)

Synthetic scheme

