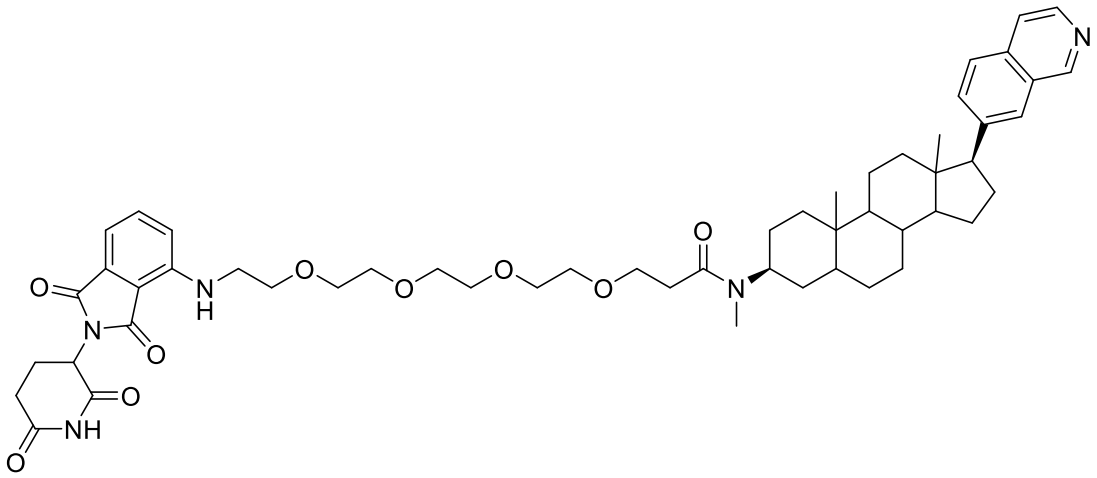
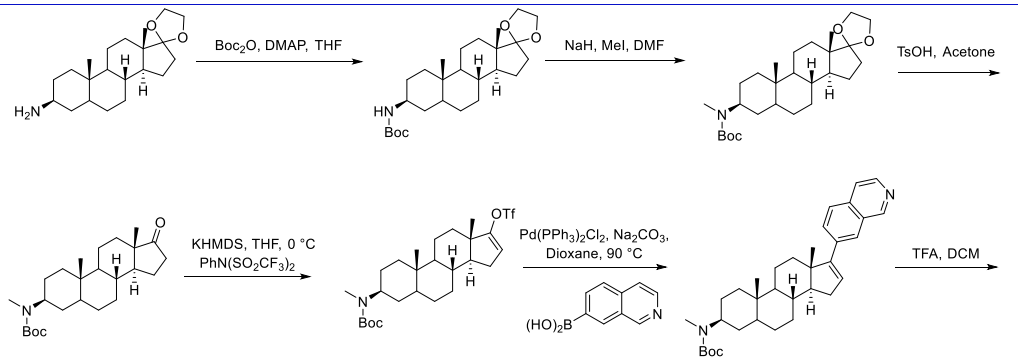
JH-XI-10-02



Chemical Formula: $C_{53}H_{69}N_5O_9$
Molecular Weight: 920.16

Category	Parameter	Description
Compound	Name	JH-XI-10-02
	Citation	*ACS Med. Chem. Lett.*, ***2018***, *9 (6), 540–545. DOI:10.1021/acsmedchemlett.8b00011*
	Chemical descriptors	CN([C@H]1CCC2(C)C(CCC3C4CC[C@H](C5=CC6=C(C=CN=C6)C=C5)C4(C)CCC23)C1)C(=O)CCOCCOCCOCCOCCNC1=C2C(=O)N(C3CCC(=O)NC3=O)C(=O)C2=CC=C1
	Chemical name	1-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisoindolin-4-yl)amino)-N-((3S,17S)-17-(isoquinolin-7-yl)-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-3-yl)-N-methyl-3,6,9,12-tetraoxapentadecan-15-amide
	Entries in chemical databases	**CID** 29937979
	Availability	None
In vitro profiling	Target (potency)	CDK8 Enzyme IC50 = 159nM. Shows complete degradation of CDK8 at a concentration of 1 µM follow treatment of 24h in Jurkatt cells
	Target (potency)	n/a
	Selectivity	
	Potential reactivity	
	SAR	
	Mechanism of inhibition	
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	JH-XI-10-02 dose-dependently inhibited pS727-Stat1 in Jurkatt cells.
	Validation of cellular specificity	
Pharmacodynamics		

Pharmacokinetics



Synthetic scheme