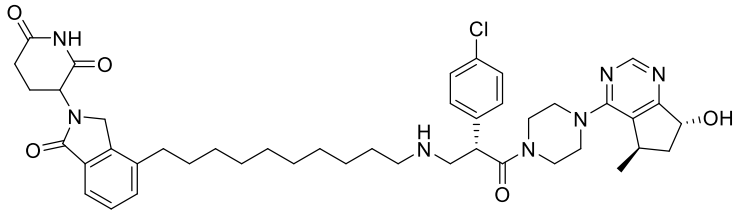
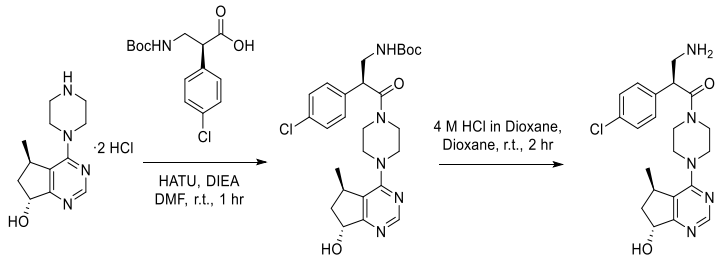
INY-03-041



Chemical Formula: $C_{44}H_{56}ClN_7O_5$
Molecular Weight: 798.43

Category	Parameter	Description
Compound	Name	INY-03-041
	Citation	Cell Chem Biol. 2019 (in press) https://doi.org/10.1016/j.chembiol.2019.11.014
	Chemical descriptors	C[C@@H]1C[C@H](C2=C1C(N3CCN(C([C@@H](C4=CC=C(C=C4)Cl)CNCCCCCCCCCCC5=CC=CC6=C5CN(C6=O)C7CCC(NC7=O)=O)=O)CC3)=NC=N2)O
	Chemical name	3-(4-(10-(((S)-2-(4-chlorophenyl)-3-(4-((5R,7R)-7-hydroxy-5-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)piperazin-1-yl)-3-oxopropyl)amino)decyl)-1-oxoisoindolin-2-yl)piperidine-2,6-dione
	Entries in chemical databases	N/A
	Availability	N/A
	Papers that use the compounds	N/A
	Additional comments	Negative control INY-03-112 also available
In vitro profiling	Target (potency)	AKT1: 2.0 nM (ZYLTE); AKT2: 6.8 nM (ZYLTE); AKT3: 3.5 nM (ZYLTE)
	Target (potency)	PKG1: 33.4 nM (ZYLTE); S6K1: 37.3 nM (ZLYTE); PKN1: 51.7 nM (ZYLTE); βMSK2: 3.3 nM (ZLYTE)
	Selectivity	KiNativ at 1 μM (AKT1, AKT2, AKT3, HASPIN, HIPK1, PKN1, PRKG1, RPS6KA4 > 70%I)
	Potential reactivity	Lenalidomide motif
	SAR	N/A
	Mechanism of inhibition	Proteasome degradation
	Structure of target-probe complex	N/A
	Additional comments	Negative control INY-03-112 was methylated on glutarimide ring based on ZNL-02-041
Cellular profiling	Validation of cellular target	Target degradation and rescue
	Validation of cellular specificity	Proteomics in MOLT4
	Additional comments	
Pharmacodynamics		N/A
Pharmacokinetics		N/A

Scheme 1



Scheme 2

Synthetic scheme