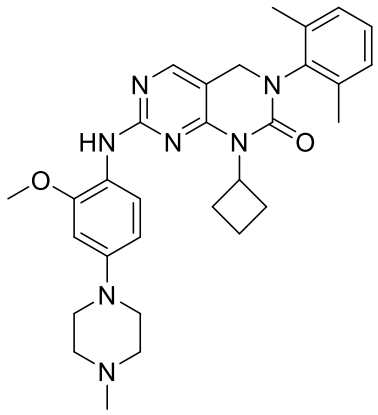
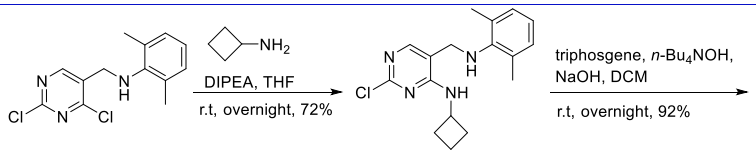
YKL-06-061



Chemical Formula: $C_{30}H_{37}N_7O_2$
Molecular Weight: 527.67

Category	Parameter	Description
Compound	Name	YKL-06-061
	Citation	*Cell Rep*. **2017**, *19*, 2177-2184. http://www.cell.com/cell-reports/fulltext/S2211-1247(17)30684-8
	Chemical descriptors	O=C(N(C1=N2)C3CCC3)N(C4=C(C=CC=C4C)C)CC1=CN=C2NC5=C(OC)C=C(N6CCN(CC6)C)C=C5
	Chemical name	1-cyclobutyl-3-(2,6-dimethylphenyl)-7-((2-methoxy-4-(4-methylpiperazin-1-yl)phenyl)amino)-3,4-dihydropyrimido[4,5-*d*]pyrimidin-2(1*H*)-one
	Entries in chemical databases	
	Availability	
	Papers that use the compounds	
In vitro profiling	Target (potency)	SIK2 (IC_{50} 1.77 nM)
	Target (potency)	SIK1 (IC_{50} 6.56 nM), SIK3 (IC_{50} 20.5 nM)
	Selectivity	S-score (1) = 0.04 (Ambit)
	Potential reactivity	
	SAR	
	Mechanism of inhibition	reversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	YKL-06-061 dose-dependently upregulates mRNA levels of MITF and TRPM1 *in vitro*.
	Validation of cellular specificity	
Pharmacodynamics		YKL-06-061 induced significant pigmentation after 8 days of topical treatment of human skin explants.
Pharmacokinetics		



Synthetic scheme