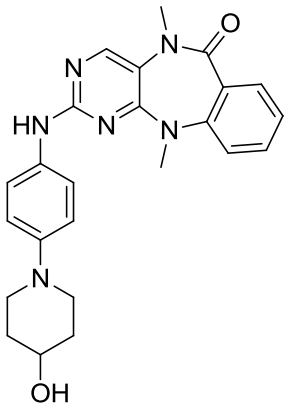
Aurora inhibitor (compound 1)



Chemical Formula: $C_{24}H_{26}N_6O_2$
Molecular Weight: 430.50

Category	Parameter	Description
Compound	Name	Aurora inhibitor (compound 1)
	Citation	*ACS. Chem. Biol.* **2011**, doi: 10.1021/cb200305u.
	Chemical descriptors	CN(C1=CN=C(NC2=CC=C(N3CCC(O)CC3)C=C2)N=C1N(C)C4=C5C=CC=C4)C5=O
	Chemical name	2-((4-(4-hydroxypiperidin-1-yl)phenyl)amino)-5,11-dimethyl-5H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6(11H)-one
	Availability	
In vitro profiling	Target (potency)	**Aurora A/B/C** (5.6/18.4/24.6 nM IC_{50} in Invitrogen biochemical assay)
	Target (potency)	**DCAMKL2** (87.7 nM IC_{50} in Invitrogen biochemical assay) **LRRK2** (30.5 nM IC_{50} in Invitrogen biochemical assay) **LRRK2(G2019S)** (10.7 nM IC_{50} in Invitrogen biochemical assay) **MAP3K2** (155 nM IC_{50} in Invitrogen biochemical assay) **MAP3K3** (120 nM IC_{50} in Invitrogen biochemical assay) **NUAK1** (52.2 nM IC_{50} in Invitrogen biochemical assay) **TAOK2** (54.3 nM IC_{50} in Invitrogen biochemical assay)
	Selectivity	
	Potential reactivity	None to our knowledge
	SAR	
	Mechanism of inhibition	ATP-competitive
	Structure of target-probe complex	3ZTX

Cellular profiling	Validation of cellular target	Compound 1 dose-dependently inhibited Aurora A autophosphorylation monitored by T288 residue in HeLa S3 cell, completely inhibited Aurora A at 250 nM. Compound 1 dose-dependently inhibited Aurora B autophosphorylation monitored by T232 residue in HeLa S3 cell, completely inhibited Aurora A at 250 nM. Compound 1 dose-dependently inhibited HCT116 cell growth with EC50 of 9.5 nM. Compound 1 dose-dependently inhibited HT29 cell growth with EC50 of 55 nM. Compound 1 dose-dependently inhibited HeLa cell growth with EC50 of 16.7 nM. Compound phenotypes were compared to literature. The cellular effects were correlated with *in vitro* biochemical activities.
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		
Synthetic scheme