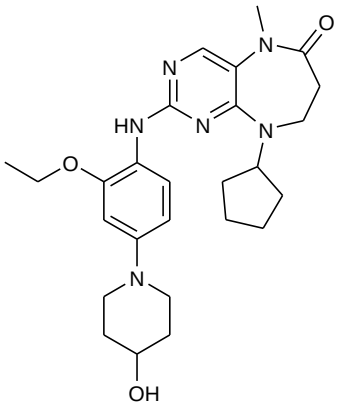
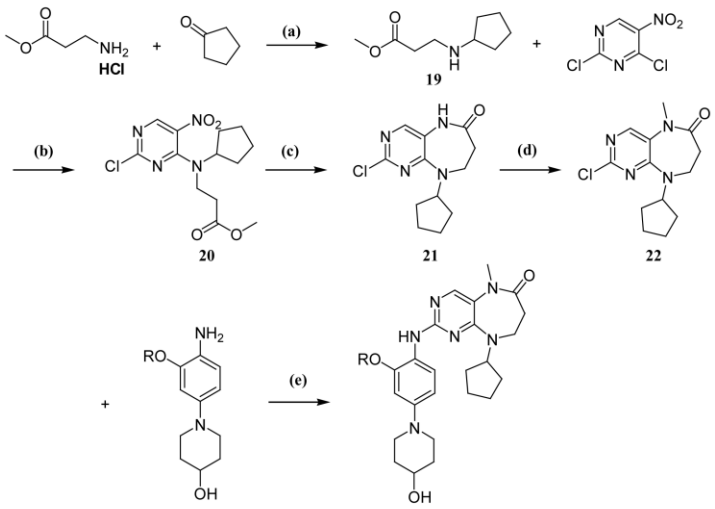
Chemical probe data: Mps1-IN-2



Chemical Formula: $C_{26}H_{36}N_6O_3$
Molecular Weight: 480.6024

Category	Parameter	Description
Compound	Name	Mps1-IN-2
	Citation	*Nat. Chem. Biol.* **2010**, 6(5), 359-68.
	Chemical descriptors	OC(CC1)CCN1C(C=C2)=CC(OCC)=C2NC3=NC=C4C(N(C5CCCC5)CCC(N4C)=O)=N3
	Chemical Name	9-cyclopentyl-2-(2-ethoxy-4-(4-hydroxypiperidin-1-yl)phenylamino)-5-methyl-8,9-dihydro-5H-pyrimido[4,5-b][1,4]diazepin-6(7H)-one
	Entries in chemical databases	Pubchem ID: 44968267
	Availability	Compound can be made available from the laboratory of Dr. Gray, DFCI and HMS
In vitro profiling	Target (potency)	Mps1 – 145 nM IC_{50} in Invitrogen biochemical assay, 12 nM K_D in Ambit binding assay
	Additional Target (potency)	Plk1 – 61 nM K_D in Ambit binding assay Gak – 140 nM K_D in Ambit binding assay
	Selectivity	*Nat. Chem. Biol.* **2010**, 6(5), 359-68, Supplementary Tables S1 and S2
	Potential reactivities	None to our knowledge
	SAR	*Nat. Chem. Biol.* **2010**, 6(5), 359-68, Supplementary Fig. S3
	Mechanism of inhibition	ATP-competitive
	Structure of the target-probe complex	3H9F (contains analog of Mps1-IN-2, *Nat. Chem. Biol.* **2010**, 6(5), 359-68, Fig. 1c, 1d, Supplementary Fig. S3 and S4, Supplementary Table S3).
Cellular profiling	Validation of cellular target	Dose-dependently inhibited spindle checkpoint at 1 μM -10 μM in Hela and U2OS cells *Nat. Chem. Biol.* **2010**, 6(5), 359-68, Fig. 2.
	Validation of cellular specificity	An inhibitor resistant mutant was developed to assess intracellular specificity. *Nat. Chem. Biol.* **2010**, 6(5), 359-68, Fig. 2.

Pharmacodynamics	Not studied.
Pharmacokinetics	Not studied.
Synthetic Scheme	



[a] Reagents and conditions: (a) NaOAc, $Na(OAc)_3BH$, DCM, room temperature, 18 h; (b) K_2CO_3, acetone, room temperature, 18h; (c) Fe, AcOH, 60°C, 4h; (d) NaH, MeI, DMA, 0°C, 4 h; (e) K_2CO_3, $Pd_2(dba)_3$, X-Phos, t-BuOH, 100°C, 5h.