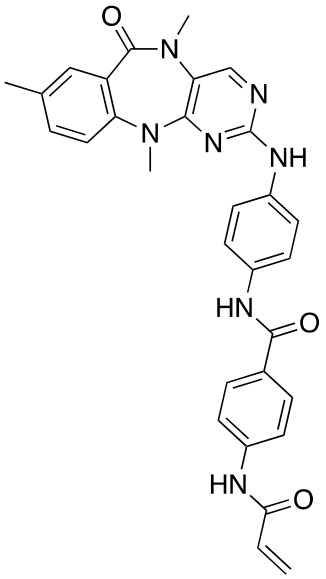
FMF-01-086-2



Chemical Formula: $C_{30}H_{27}N_7O_3$
Molecular Weight: 533.59

Category	Parameter	Description
Compound	Name	FMF-01-086-2
	Citation	Bioorg Med Chem Lett. 2017 Sep 15;27(18):4405-4408. https://doi.org/10.1016/j.bmcl.2017.08.016
	Chemical descriptors	CC1=CC2=C(N(C)C(N=C(NC3=CC=C(NC(C4=CC=C(NC(C=C)=O)C=C4)=O)C=C3)N=C5)=C5N(C)C2=O)C=C1
	Chemical name	4-acrylamido-*N*-(4-((5,8,11-trimethyl-6-oxo-6,11-dihydro-5*H*-benzo[*e*]pyrimido[5,4-*b*][1,4]diazepin-2-yl)amino)phenyl)benzamide
	Entries in chemical databases	
	Availability	
	Papers that use the compounds	
	Additional comments	
In vitro profiling	Target (potency)	Aurora A (IC_{50} = 44 nM +/- 4.5 nM)
	Target (potency)	Aurora B (IC_{50} = 29 nM +/- 2.0 nM)
	Target (potency)	Aurora C (IC_{50} = 63 nM +/- 8.1 nM)
	Selectivity	Exclusively on-target activity detected by KINOME*scan* ® at 1 μ M compound concentration. PLK4 biochemical IC_{50} = 43 nM
	Potential reactivity	Cysteine reactive
	SAR	Described in paper
	Mechanism of inhibition	Reversible
	Structure of target-probe complex	

Cellular profiling	Validation of cellular target	Dose dependent inhibition of pAurora A (Aurora A substrate) and pH3 S10 (Aurora B substrate) in HCT116 cells. Effects on cell cycle consistent with selective on-target inhibition.
	Validation of cellular specificity	
Pharmacodynamics		n/a
Pharmacokinetics		n/a
Synthetic scheme