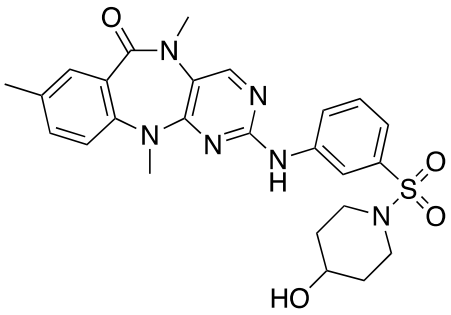
FMF-02-063-1



Chemical Formula: $C_{25}H_{28}N_6O_4S$
Molecular Weight: 508.60

Category	Parameter	Description
Compound	Name	FMF-02-063-1
	Citation	ACS Med Chem Lett. 2016 Aug 2;7(10):908-912 **DOI:** 10.1021/acsmedchemlett.6b00209
	Chemical descriptors	CC1=CC2=C(N(C)C(N=C(NC3=CC(S(=O)(N4CCC(O)CC4)=O)=CC=C3)N=C5)=C5N(C)C2=O)C=C1
	Chemical name	2-((3-((4-hydroxypiperidin-1-yl)sulfonyl)phenyl)amino)-5,8,11-trimethyl-5,11-dihydro-6*H*-benzo[*e*]pyrimido[5,4-*b*][1,4]diazepin-6-one
	Entries in chemical databases	
	Availability	
	Papers that use the compounds	
In vitro profiling	Target (potency)	PI3K-δ IC_{50} = 2.1 nM +/- 0.68 nM
	Target (potency)	PI3K-γ IC_{50} = 6.5 nM +/- 1.5 nM
	Selectivity	On target activity + Aurora activity detected by KINOME*scan*® at 1 μ M compound concentration. PI3K-α IC_{50} =55 nM +/- 16 nM PI3K-β IC_{50} = 4800 nM +/- 9500 nM Aurora A IC_{50} = 150 nM +/- 6.3 nM Aurora B IC_{50} = 150 nM +/- 38 nM
	Potential reactivity	
	SAR	Described in paper
	Mechanism of inhibition	Reversible
	Structure of target-probe complex	ND
Cellular profiling	Validation of cellular target	Inhibits p308 AKT and p473 AKT signaling in isogenic HMEC cell lines where PI3K signaling is driven exclusively by CA-p110-δ under serum starved conditions,
	Validation of cellular specificity	Does not inhibit p308 AKT and p473 AKT signaling in isogenic HMEC cell lines where PI3K signaling is driven exclusively by CAp110-α or CA-p110-β.

Pharmacodynamics	ND
Pharmacokinetics	ND
Synthetic scheme