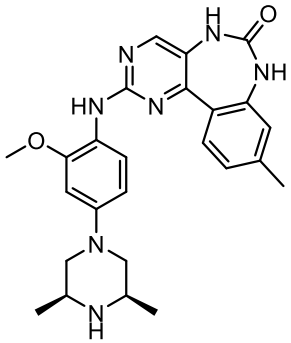
SYN-DFCI-00114



Chemical Formula: $C_{25}H_{29}N_7O_2$
Molecular Weight: 459.55

Category	Parameter	Description
Compound	Name	SYN-DFCI-00114 (compound 32 in reference paper)
	Citation	Bioorg Med Chem Lett 30(19): 127456 https://doi.org/10.1016/j.bmcl.2020.127456
	Chemical descriptors	O=C(NC1=C(C2=N3)C=CC(C)=C1)NC2=CN=C3NC4=C(OC)C=C(N5C[C@H](C)N[C@H](C)C5)C=C4
	Chemical name	2-((4-((3S,5R)-3,5-dimethylpiperazin-1-yl)-2-methoxyphenyl)amino)-9-methyl-5,7-dihydro-6H-benzo[d]pyrimido[4,5-f][1,3]diazepin-6-one
	Entries in chemical databases	N/A
	Availability	N/A
	Additional comments	N/A
In vitro profiling	Target (potency)	TNK2/ACK1: 102 nM (Lantha screen)
	Selectivity	KINOMEscan at 1 µM (TNK2, GAK, SRMS, Abl)<5%
	Potential reactivity	GAK, SRMS, Abl
	SAR	Described in this paper
	Mechanism of inhibition	Type I ATP competitive inhibitor
	Structure of target-probe complex	TNK2 co-crystal structure (PDB: 6VPM)
	Additional comments	N/A
Cellular profiling	Validation of cellular target	TNK2 D163E Ba/F3 cells
	Validation of cellular specificity	N/A
	Additional comments	
Pharmacodynamics		N/A
Pharmacokinetics		Cl (ml/min/kg) IV T1/2 (hr) F % Auc inf (PO) (ng*hr/ml) 77 1.8 9 200

Synthetic scheme