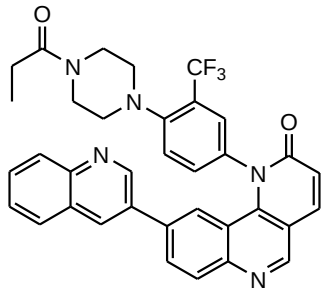
Torin 1



Chemical Formula: $C_{35}H_{28}F_3N_5O_2$
Molecular Weight: 607.62

Category	Parameter	Description
Compound	Name	Torin 1
	Citation	*J Med Chem*. **2010**, *53(19),* 7146-55.
	Chemical descriptors	O=C1N(C2=CC(C(F)(F)F)=C(N3CCN(C(CC)=O)CC3)C=C2)C4=C(C=C1)C=NC5=CC=C(C6=CN=C(C=CC=C7)C7=C6)C=C54
	Chemical name	1-(4-(4-propionylpiperazin-1-yl)-3-(trifluoromethyl)phenyl)-9-(quinolin-3-yl)benzo[h][1,6]naphthyridin-2(1H)-one
	Availability	Tocris Bioscience http://www.tocris.com/dispprod.php?ItemId=294888
In vitro profiling	Primary target (potency)	**mTORC1** (IC_{50} of 0.29 nM)
	Other target (potency)	Invitrogen Lipid Kinase panel: **PI4K β** (IC_{50} of 6680 nM), **PI3K-C2α** (IC_{50} of 176 nM), **PI3K-C2β** (IC_{50} of 549 nM), **hVPS34** (IC_{50} of 533 nM), **P110 α/p85α** (IC_{50} of 250 nM), **P110δ/P85α** (IC_{50} of 564 nM), **P110γ** (IC_{50} of 171 nM), **DNA-PK** (IC_{50} of 6.34 nM)
	Selectivity	Torin1 is extremely selective for PIKKfamily kinases relative to all other serine/threonine and tyrosine kinases. Torin1 is very selective relative to other PIKK family kinases with the exception of DNA-PK.
	Potential reactivity	
	SAR	*J Med Chem*. **2010**, *53(19),* 7146-55, Table 3, 4 and 5.
	Mechanism of inhibition	ATP-competitive
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	
	Validation of cellular specificity	800-fold selectivity over PI3K
Pharmacodynamics		

Pharmacokinetics

Route	C_{max} (ng/mL)	T_{max} (h)	AUC (h*ng/mL)	$T_{1/2}$ (h)	MRT (h)	CL (mL/min/Kg)	V_{ss} (L/Kg)	F (%)
IV	2757	ND	720	0.5	0.43	23.0	0.59	ND
PO	223	0.25	396	0.79	1.51	ND	ND	5.49
IP	5121	0.08	5718	4.52	ND	ND	ND	ND

Synthetic scheme