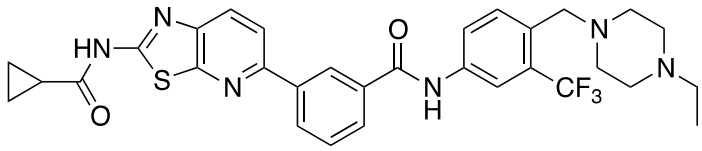
HG-7-85-01



Chemical Formula: $C_{31}H_{31}F_3N_6O_2S$
Exact Mass: 608.22

Category	Parameter	Description
Compound	Name	HG-7-85-01
	Citation	*Blood*, 2010, 115(21), 4206-4216, *Mol Cancer Ther* 2010 9,2468-2477
	Chemical descriptors	O=C(C1CC1)NC(S2)=NC3=C2N=C(C4=CC=CC(C(NC5=CC(C(F)(F)F)=C(CN6CCN(CC)CC6)C=C5)=O)=C4)C=C3
	Chemical name	3-(2-(cyclopropanecarboxamido)thiazolo[5,4-*b*]pyridin-5-yl)-*N*-(4-((4-ethylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)benzamide
In vitro profiling	Target (potency)	Abl1 IC_{50} 28.2 nM, Abl1(T315I) IC_{50} 36.6 nM, FLT3 IC_{50} 12.2 nM, RET IC_{50} 52.7 nM VEGFR2 IC_{50} 60.7 nM, and PDGFRB IC_{50} 680 nM (Invitrogen biochemical assay)
	Additional Target (potency)	EGFR, Tie-2, JAK1, Kit, Src, DDR1, and b-Raf,
	Selectivity	
	Potential reactivity	None to our knowledge
	SAR	
	Mechanism of inhibition	ATP-competitive type II inhibitor
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	Bcr-Abl IC_{50} 60 nM, BCR-ABL-T315I IC_{50}140 nM, Kit-T670I IC_{50} 250 nM, PDGFRα-T674M IC_{50}6.25 nM, and PDGFRα-T674I IC_{50} 6.25 nM (Ba/F3 cell lines)
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		$T_{1/2}$ mouse =1.1 h rat = 5.8 hours, Cmax mouse = 106 ng/mL at 10 mg/kg , rat = 292 ng/mL and 2 mg/kg, CL mouse = 23 ml/min/kg, rat = 13 ml/min/kg, F = mouse = 5 %, rat = 19 %

Synthetic scheme