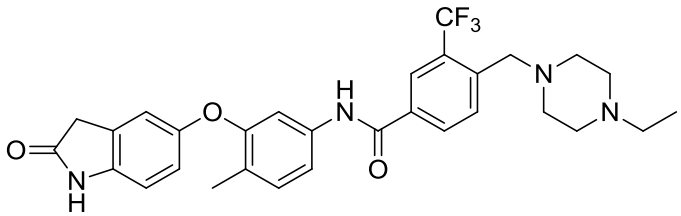
DDR1 inhibitor (DDR-IN-1)



Chemical Formula: $C_{30}H_{31}F_3N_4O_3$
Molecular Weight: 552.59

Category	Parameter	Description
Compound	Name	DDR1 inhibitor (DDR-IN-1)
	Citation	*ACS Chem Biol*. 2013 Aug. **DOI:** 10.1021/cb400430t
	Chemical descriptors	O=C(N1)CC2=C1C=CC(OC3=C(C)C=CC(NC(C4=CC=C(CN5CCN(CC)CC5)C(C(F)(F)F)=C4)=O)=C3)=C2
	Chemical name	4-((4-ethylpiperazin-1-yl)methyl)-*N*-(4-methyl-3-((2-oxoindolin-5-yl)oxy)phenyl)-3-(trifluoromethyl)benzamide
	Availability	
In vitro profiling	Target (potency)	**DDR1** (105 nM IC50 in Invitrogen binding assay (LanthaScreen))
	Target (potency)	**DDR2** (413 nM IC50 in Invitrogen binding assay (LanthaScreen))
	Selectivity	
	Potential reactivity	None to our knowledge
	SAR	
	Mechanism of inhibition	ATP-competitive
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	DDR-IN-1 dose-dependently inhibited DDR1 autophosphorylation induced by collagen in U2OS cells with IC50 of 84 nM.
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		$T_{1/2}$ = 2.76 hours, CL = 89.88 (mL/min/Kg), Vss = 18.02 (L/Kg), F = 26%

Synthetic scheme