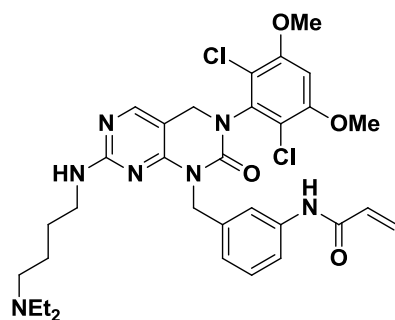


FIIN-1



Chemical Formula: $C_{32}H_{39}Cl_2N_7O_4$

Molecular Weight: 656.60

Category	Parameter	Description
Compound	Name	FIIN-1
	Citation	<i>Chemistry & Biology</i> 2010 , 17(3), 285-95
	Chemical descriptors	<chem>O=C1N(CC2=CC=CC(NC(C=C)=O)=C2)C3=NC(NCCCCN(CC)CC)=NC=C3CN1C4=C(Cl)C(OC)=CC(OC)=C4Cl</chem>
	Chemical name	N-(3-((3-(2,6-dichloro-3,5-dimethoxyphenyl)-7-((4-(diethylamino)butyl)amino)-2-oxo-3,4-dihydropyrimido[4,5-d]pyrimidin-1(2H)-yl)methyl)phenyl)acrylamide
	Entries in chemical databases	CID 53348188
	Availability	
<i>In vitro</i> profiling	Target (potency)	FGFR1, 2, 3, 4 (IC50= 9.2, 6.2, 11.9, 189 nM in biochemical assay) FGFR1, 2, 3, 4 (IC50= 2.8, 6.9, 5.4, 120 nM in Ambit binding assay)
	Target (potency)	BLK (Kd=65 nM in Ambit binding assay) FLT1 (Kd=32 nM in Ambit binding assay)
	Selectivity	
	Potential reactivity	Cysteine reactive
	SAR	
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	FIIN-1 dose-dependently inhibited the activation of FGFR and its downstream signals in the inducible FGFR1 MCF10A cells at 20 nM A biotin-labeled FIIN-1 demonstrated the binding of FIIN-1 to FGFRs. FIIN-1 abolished iFGFR-1 mediated mammary epithelial cell transformation in 3D cells
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		

Synthetic scheme

