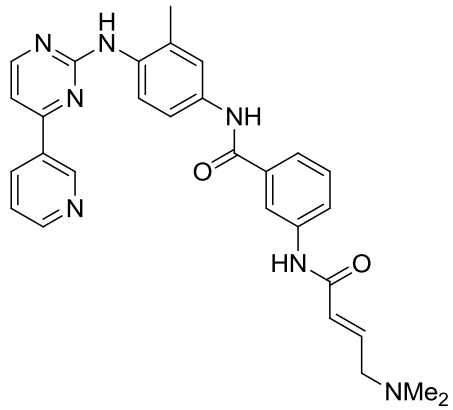
JNK-IN-8



Chemical Formula: $C_{29}H_{29}N_7O_2$
Molecular Weight: 507.59

Category	Parameter	Description
Compound	Name	JNK-IN-8
	Citation	*Chemistry& Biology* **2012**, *19(1):*140-154
	Chemical descriptors	CC1=CC(NC(C2=CC(NC(/C=C/CN(C)C)=O)=CC=C2)=O)=CC=C1NC3=NC=CC(C4=CN=CC=C4)=N3
	Chemical name	(*E*)-3-(4-(dimethylamino)but-2-enamido)-*N*-(3-methyl-4-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)benzamide
In vitro profiling	Primary target (potency)	**JNK1** (IC_{50}: 4.67 nM) JNK2 (IC_{50}: 18.7 nM) JNK3 (IC_{50}: 0.98 nM)
	Other target (potency)	MNK2 (IC_{50}: 238 nM) FMS (IC_{50}: 287 nM) KIT(V559D) (Kd 92 nM) KIT(V559D,T670I) (Kd 56 nM) PRKX (Ambit score 0) HIPK4 (Ambit score 4) PDGFRB (Ambit score 4.7)
	Selectivity	JNK-IN-8 exhibit excellent overall selectivity Cellular kinase profiling with KiNative technology showed JNK-IN-8 only target JNKs among the other more than 200 kinases. In Vitro profiling with ambit also showed a high selective S score for JNK-IN-8 (0.031)
	SAR	*Chemistry& Biology* **2012**, *19(1):*140-154
	Mechanism of inhibition	JNK-IN-8 is an irreversible JNK1/2/3 inhibitor which forms a covalent bond with cys 116 on JNK1 and JNK2 and with cys 154 on JNK3
	Structure of target-probe complex	3V6S
Cellular activity	JNK-IN-8 inhibit c-Jun phosphorylation on cells with a IC_{50} of 300 – 500 nM	

Synthetic scheme