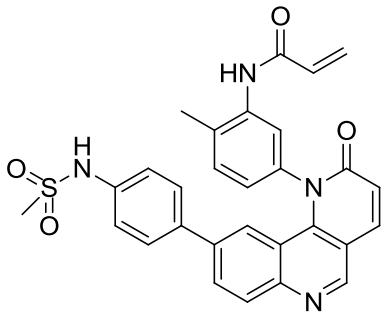
BMX-IN-1



Chemical Formula: $C_{29}H_{24}N_4O_4S$
Molecular Weight: 524.59

Category	Parameter	Description
Compound	Name	BMX-IN-1
	Citation	*ACS Chem Biol.* ***2013***
	Chemical descriptors	CC(C=C1)=C(NC(C=C)=O)C=C1N2C3=C(C=CC2=O)C=NC4=CC=C(C5=CC=C(NS(=O)(C)=O)C=C5)C=C43
	Chemical name	N-(2-methyl-5-(9-(4-(methylsulfonamido)phenyl)-2-oxobenzo[h][1,6]naphthyridin-1(2H)-yl)phenyl)acrylamide
	Entries in chemical databases	
	Availability	
In vitro profiling	Target (potency)	BMX (8.0 nM, Invitrogen SelectScreen)
	Additional Target (potency)	BTK (10.4 nM, Invitrogen SelectScreen)
	Selectivity	Selectivity profiling against a panel of 442 kinases using the KinomeScan approach at a concentration of 1 uM revealed that BMX-IN-1 exhibited remarkable selectivity with an S(10) score of 0.01
	Potential reactivity	Cysteine reactive
	SAR	
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	inhibited Tel-BMX-transformed Ba/F3 cells at 25 nM
	Validation of cellular specificity	discriminate among Tec family kinases
Pharmacodynamics		
Pharmacokinetics		

Synthetic scheme