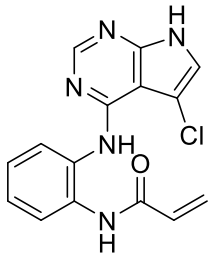
BSJ-04-122



Chemical Formula: $C_{15}H_{12}ClN_5O$
Molecular Weight: 313.75

Category	Parameter	Description
Compound	Name	BSJ-04-122
	Citation	Cell Chemical Biology 2020, 27, 1553–1560
	Chemical descriptors	ClC1=CNC2=C1C(NC1=C(NC(=O)C=C)C=CC=C1)=NC=N2
	Chemical name	N-(2-((5-chloro-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)phenyl)acrylamide
	Entries in chemical databases	
	Availability	
In vitro profiling	Target (potency)	BSJ-04-122 Is a Covalent MKK4 and MKK7 Inhibitor, MKK4 (4nM)
	Target (potency)	
	Selectivity	MKK4 and MKK7 are the top targets bound by BSJ-04-122 in MDA-MB-231 cells pretreated with the compound for 6 h (with 90.2% and 87.0%, respectively), whereas most protein kinases were not affected.
	Potential reactivity	Cyeteine reactive
	SAR	
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	BSJ-04-122 significantly decreased levels of T183/Y185 pJNK at 5 mM, resulting in complete inhibition at 10 mM. No effect on the phosphorylation of p38, a downstream effector of MKK3/6. Similarly, the MKK1/2 and MKK5 pathways were also not inhibited, as assessed by phosphorylation levels of downstream substrates ERK1/2 and ERK5.
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		

Synthetic scheme