### BSJ-04-122

![Chemical Structure](image)

- **Chemical Formula:** $\text{C}_{15}\text{H}_{12}\text{ClN}_{5}\text{O}$
- **Molecular Weight:** 313.75

#### Category | Parameter | Description
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**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) | 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.
 | Selectivity | 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

\[ \text{DIPEA, NMP, 140}^\circ \text{C} \]

\[ \text{DIPEA, Acetonitrile, 0}^\circ \text{C} \]