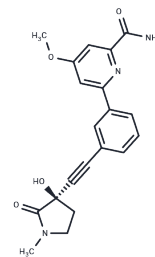


## NIK SMI1

## Chemical Properties

|                   |   |
|-------------------|---|
| CAS No. :         | 1660114-31-7  |
| Formula:          | C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> |
| Molecular Weight: | 365.38  |
| Appearance:       | no data available   |
| Storage:          | Powder: -20°C for 3 years   In solvent: -80°C for 1 year      |



## Biological Description

|                            |  |
|----------------------------|--|
| Description                | NIK SMI1 is an effective and selective NF-κB inducing kinase (NIK) inhibitor. It also inhibits NIK-catalyzed hydrolysis of ATP to ADP (IC <sub>50</sub> : 0.23±0.17 nM).   |
| Targets(IC <sub>50</sub> ) | NF-κB  |
| In vitro                   | NIK SMI1 inhibits the expression of NIK SMI1 response element regulated firefly luciferase reporter gene in HEK293 cells (IC <sub>50</sub> : 34±6 nM). NIK SMI1 inhibits BAFF-induced B cell (mouse) survival in vitro with an IC <sub>50</sub> of 373±64 nM. Consistent with expectations for a NIK inhibitor, NIK SMI1 is shown to inhibit nuclear translocation of p52 (RelB) (IC <sub>50</sub> =70 nM).  |
| In vivo                    | The pharmacology of NIK SMI1 is examined in SD rat, CD-1 mouse, beagle, and cynomolgous monkey with 20, 32, 18, and 7.8 mL/kg per min, respectively. The volume of distribution (V <sub>d</sub> , L/kg) is 1.35, 1.58, 0.778, and 1.39, respectively. C57BL/6 mice are treated twice daily for 7 days with orally administered NIK SMI1 or with three injections of recombinant BAFF receptor fusion protein (Br3- mIgG2a) over the course of the 7-day experiment as a positive control . |

## Solubility Information

|            |   |
|------------|---|
| Solubility | DMSO: 100 mg/mL (273.69 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
|------------|---|

## A DRUG SCREENING EXPERT

### Preparing Stock Solutions

|       | 1mg       | 5mg        | 10mg       |
|-------|-----------|------------|------------|
| 1 mM  | 2.7369 mL | 13.6844 mL | 27.3688 mL |
| 5 mM  | 0.5474 mL | 2.7369 mL  | 5.4738 mL  |
| 10 mM | 0.2737 mL | 1.3684 mL  | 2.7369 mL  |
| 50 mM | 0.0547 mL | 0.2737 mL  | 0.5474 mL  |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

### Reference

Blaquiere N, et al. Scaffold-Hopping Approach To Discover Potent, Selective, and Efficacious Inhibitors of NF- $\kappa$ B Inducing Kinase. J Med Chem. 2018 Aug 9;61(15):6801-6813.

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