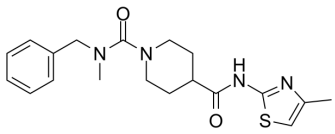
# H3B-120

| | |
|---|---|
| **Cat. No.:** | HY-136128 |
| **CAS No.:** | 2194903-42-7 |
| **Molecular Formula:** | $C_{19}H_{24}N_4O_2S$ |
| **Molecular Weight:** | 372.48 |
| **Target:** | Potassium Channel |
| **Pathway:** | Membrane Transporter/Ion Channel |
| **Storage:** | Powder -20°C 3 years<br>4°C 2 years<br>In solvent -80°C 2 years<br>-20°C 1 year |



## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : 62.5 mg/mL (167.79 mM; Need ultrasonic)

| Preparing Stock Solutions | Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|---|
| | 1 mM | 2.6847 mL | 13.4235 mL | 26.8471 mL |
| | 5 mM | 0.5369 mL | 2.6847 mL | 5.3694 mL |
| | 10 mM | 0.2685 mL | 1.3424 mL | 2.6847 mL |

Please refer to the solubility information to select the appropriate solvent.

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (5.58 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.58 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.58 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

H3B-120 is a highly selective, competitive and allosteric carbamoyl phosphate synthetase 1 (CPS1) inhibitor with an $IC_{50}$ of 1.5 μM and a $K_i$ of 1.4 μM. H3B-120 has anti-cancer activity[1].

**$IC_{50}$ & Target**

IC50: 1.5 μM (CPS1)[1]
Ki: 1.4 μM (CPS1)[1]

**In Vitro**

H3B-120 has no inhibition of CPS2 activity of CAD (CPS2, aspartyl transcarbamylase, dihydroorotase)[1].

H3B-120 achieves inhibition by binding to an allosteric pocket situated between the integrating and ATP A domains[1].
H3B-120 (25, 50, 75, 100 μM) inhibits urea production in a dose-dependent manner, although the cellular potency decreases significantly compared with enzymatic assays[1].
The half-life of H3B-120 is only 40 min[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## REFERENCES

[1]. Yao S, et al. Small Molecule Inhibition of CPS1 Activity through an Allosteric Pocket. Cell Chem Biol. 2020 Mar 19;27(3):259-268.



Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA