H3B-120

Cat. No.: HY-136128

CAS No.: 2194903-42-7

Molecular Formula: $C_{19}H_{24}N_4O_2S$

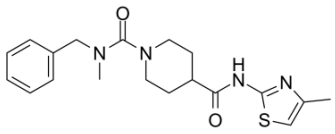
Molecular Weight: 372.48

Target: Potassium Channel

Pathway: Membrane Transporter/Ion Channel

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



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.

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