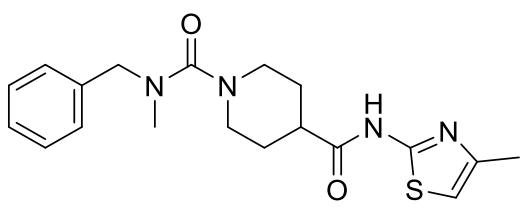


# Product data sheet



MedKoo Cat#: 462455 Name: H3B-120 CAS: 2194903-42-7 Chemical Formula: C <sub>19</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub> S Exact Mass: 372.162 Molecular Weight: 372.487	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

## 1. Product description:

H3B-120 is a highly selective, competitive and allosteric carbamoyl phosphate synthetase 1 (CPS1) inhibitor that has anti-cancer activity.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	68.75	184.57
Ethanol	19.0	51.01

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.68 mL	13.42 mL	26.85 mL
5 mM	0.54 mL	2.68 mL	5.37 mL
10 mM	0.27 mL	1.34 mL	2.68 mL
50 mM	0.05 mL	0.27 mL	0.54 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Yao S, Nguyen TV, Rolfe A, Agrawal AA, Ke J, Peng S, Colombo F, Yu S, Bouchard P, Wu J, Huang KC, Bao X, Omoto K, Selvaraj A, Yu L, Ioannidis S, Vaillancourt FH, Zhu P, Larsen NA, Bolduc DM. Small Molecule Inhibition of CPS1 Activity through an Allosteric Pocket. Cell Chem Biol. 2020 Mar 19;27(3):259-268.e5. doi: 10.1016/j.chembiol.2020.01.009. Epub 2020 Feb 3. PMID: 32017919.

In vivo study

TBD

## 7. Bioactivity

Biological target:

H3B-120 is a highly selective, competitive and allosteric carbamoyl phosphate synthetase 1 (CPS1) inhibitor with an IC<sub>50</sub> of 1.5 μM and a K<sub>i</sub> of 1.4 μM. H3B-120 has anti-cancer activity.

In vitro activity

H3B-120 was able to inhibit urea production in a dose-dependent manner, although the cellular potency decreased significantly compared with enzymatic assays (Figure 6A).

# Product data sheet



Reference: Cell Chem Biol. 2020 Mar 19;27(3):259-268.e5. <https://pubmed.ncbi.nlm.nih.gov/32017919/>

In vivo activity

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TBD

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*