

# Product data sheet



MedKoo Cat#: 406601 Name: JIB-04 CAS: 199596-05-9 Chemical Formula: C <sub>17</sub> H <sub>13</sub> ClN <sub>4</sub> Exact Mass: 308.0829 Molecular Weight: 308.769	
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:

JIB-04, also known as NSC 693627, is a Jumonji histone demethylase inhibitor. JIB-04 selectively blocks cancer cell growth in vitro and diminishes tumor growth in H358 and A549 mouse xenograft models in vivo. JIB-04 can prolong survival in a mouse model of breast cancer.

## 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
DMF	20.0	64.77
DMSO	36.97	119.73
Ethanol	1.5	4.86

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.24 mL	16.19 mL	32.39 mL
5 mM	0.65 mL	3.24 mL	6.48 mL
10 mM	0.32 mL	1.62 mL	3.24 mL
50 mM	0.07 mL	0.32 mL	0.65 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

- Lee J, Kim JS, Cho HI, Jo SR, Jang YK. JIB-04, a Pan-Inhibitor of Histone Demethylases, Targets Histone-Lysine-Demethylase-Dependent AKT Pathway, Leading to Cell Cycle Arrest and Inhibition of Cancer Stem-Like Cell Properties in Hepatocellular Carcinoma Cells. *Int J Mol Sci.* 2022 Jul 11;23(14):7657. doi: 10.3390/ijms23147657. PMID: 35887001; PMCID: PMC9322929.
- He Y, Yi X, Zhang Z, Luo H, Li R, Feng X, Fang ZM, Zhu XH, Cheng W, Jiang DS, Zhao F, Wei X. JIB-04, a histone demethylase Jumonji C domain inhibitor, regulates phenotypic switching of vascular smooth muscle cells. *Clin Epigenetics.* 2022 Aug 13;14(1):101. doi: 10.1186/s13148-022-01321-8. PMID: 35964071; PMCID: PMC9375951.

### In vivo study

- Son J, Huang S, Zeng Q, Bricker TL, Case JB, Zhou J, Zang R, Liu Z, Chang X, Darling TL, Xu J, Harastani HH, Chen L, Gomez Castro MF, Zhao Y, Kohio HP, Hou G, Fan B, Niu B, Guo R, Rothlauf PW, Bailey AL, Wang X, Shi PY, Martinez ED, Brody SL, Whelan SPJ, Diamond MS, Boon ACM, Li B, Ding S. JIB-04 Has Broad-Spectrum Antiviral Activity and Inhibits SARS-CoV-2 Replication and Coronavirus Pathogenesis. *mBio.* 2022 Jan 18;13(1):e0337721. doi: 10.1128/mbio.03377-21. Epub ahead of print. PMID: 35038906; PMCID: PMC8764536.

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2. Parrish JK, McCann TS, Sechler M, Sobral LM, Ren W, Jones KL, Tan AC, Jedlicka P. The Jumonji-domain histone demethylase inhibitor JIB-04 deregulates oncogenic programs and increases DNA damage in Ewing Sarcoma, resulting in impaired cell proliferation and survival, and reduced tumor growth. *Oncotarget*. 2018 Sep 4;9(69):33110-33123. doi: 10.18632/oncotarget.26011. PMID: 30237855; PMCID: PMC6145692.

## 7. Bioactivity

### Biological target:

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JIB-04 is a pan-selective Jumonji histone demethylase inhibitor with IC<sub>50</sub>s of 230, 340, 855, 445, 435, 1100, and 290 nM for JARID1A, JMJD2E, JMJD3, JMJD2A, JMJD2B, JMJD2C, and JMJD2D, respectively.

### In vitro activity

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Compared with DMSO-treated controls, all the JIB-04-treated HCC cells showed increased G<sub>1</sub>-phase subpopulations and decreased G<sub>2</sub>/M-phase subpopulations (Figure 1B), suggesting the occurrence of G<sub>1</sub>/S arrest in JIB-04-treated HCC cells. Thus, these data suggested that the reduced cell viability in JIB-04-treated HCC cells might be partly caused by JIB-04-induced cell cycle defects.

Reference: *Int J Mol Sci*. 2022 Jul 11;23(14):7657. <https://pubmed.ncbi.nlm.nih.gov/35887001/>

### In vivo activity

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JIB-04 administration also ameliorated the damage of GI epithelium in TGEV-infected animals (Fig. 5D), with fewer viral antigen-positive cells (Fig. S5D). Taken together, these data demonstrate in vivo antiviral activity of JIB-04 against a porcine coronavirus.

Reference: *mBio*. 2022 Jan 18;13(1):e0337721. <https://pubmed.ncbi.nlm.nih.gov/35038906/>

*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.*