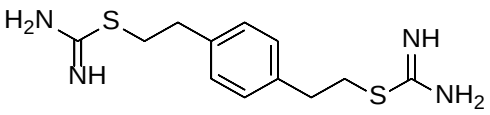
Product data sheet

MedKoo Cat#: 406515 Name: 1,4-PBIT (dihydrobromide) CAS: 157254-60-9 Chemical Formula: $C_{12}H_{18}N_4S_2$ Exact Mass: 282.0973 Molecular Weight: 282.424	
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:
1,4-PBIT (dihydrobromide) is a potent inhibitor of iNOS and nNOS with Ki values of 7.4 and 16 nM, respectively. Its inhibition in whole cells is greatly diminished, presumably to poor membrane permeability.

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	70.82
DMSO	25.0	88.52
PBS (pH 7.2)	5.0	17.70

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.54 mL	17.70 mL	35.41 mL
5 mM	0.71 mL	3.54 mL	7.08 mL
10 mM	0.35 mL	1.77 mL	3.54 mL
50 mM	0.07 mL	0.35 mL	0.71 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. Wang Q, He H, Chen D, Wang C, Xu Y, Song W. Hepatic stroma-educated regulatory DCs suppress CD8+ T cell proliferation in mice. Oncotarget. 2017 Jun 13;8(55):93414-93425. doi: 10.18632/oncotarget.18459. PMID: 29212160; PMCID: PMC5706806.
2. Sayegh J, Cao J, Zou MR, Morales A, Blair LP, Norcia M, Hoyer D, Tackett AJ, Merkel JS, Yan Q. Identification of small molecule inhibitors of Jumonji AT-rich interactive domain 1B (JARID1B) histone demethylase by a sensitive high throughput screen. J Biol Chem. 2013 Mar 29;288(13):9408-17. doi: 10.1074/jbc.M112.419861. Epub 2013 Feb 13. PMID: 23408432; PMCID: PMC3611010.

In vivo study

1. Chen T, Nines RG, Peschke SM, Kresty LA, Stoner GD. Chemopreventive effects of a selective nitric oxide synthase inhibitor on carcinogen-induced rat esophageal tumorigenesis. Cancer Res. 2004 May 15;64(10):3714-7. doi: 10.1158/0008-5472.CAN-04-0302. PMID: 15150132.

7. Bioactivity
Biological target:
1,4-PBIT (dihydrobromide) is a potent inhibitor of iNOS and nNOS with Ki values of 7.4 and 16 nM.

Product data sheet

In vitro activity

More importantly, this study identified several novel inhibitors, including 2-4(4-methylphenyl)-1,2-benzisothiazol-3(2H)-one (PBIT), which inhibits JARID1B with an IC50 of about 3 μm in vitro. Consistent with this, PBIT treatment inhibited removal of H3K4me3 by JARID1B in cells. Furthermore, this compound inhibited proliferation of cells expressing higher levels of JARID1B.

Reference: J Biol Chem. 2013 Mar 29;288(13):9408-17. https://pubmed.ncbi.nlm.nih.gov/23408432/

In vivo activity

PBIT reduced the incidence of esophageal cancer from 96% in NMBA-treated rats to 83% and 77% ($P < 0.05$) in rats treated with 50 and 100 ppm PBIT, respectively. Tumor multiplicity was reduced from 3.64 +/- 0.42 tumors per esophagus in NMBA-treated rats to 1.79 +/- 0.25 ($P < 0.001$) and 1.50 +/- 0.24 ($P < 0.0001$) in rats treated with 50 and 100 ppm PBIT, respectively. PBIT reduced the production of NO in NMBA-induced preneoplastic and papillomatous esophageal lesions when compared with comparable lesions in rats treated with NMBA only.

Reference: Cancer Res. 2004 May 15;64(10):3714-7. https://pubmed.ncbi.nlm.nih.gov/15150132/

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.