

# Product data sheet



MedKoo Cat#: 555912 Name: DTHIB CAS: 897326-30-6 Chemical Formula: C <sub>13</sub> H <sub>9</sub> ClFN <sub>3</sub> O <sub>3</sub> Exact Mass: 309.0316 Molecular Weight: 309.6814		
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:

DTHIB is a direct and selective heat shock factor 1 (HSF1) inhibitor with a K<sub>d</sub> of 160 nM. DTHIB physically engages HSF1 and selectively stimulates degradation of nuclear HSF1.

## 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	93.0	300.31
Ethanol	17.0	54.90

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.23 mL	16.15 mL	32.29 mL
5 mM	0.65 mL	3.23 mL	6.46 mL
10 mM	0.32 mL	1.61 mL	3.23 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

1. Dong B, Jaeger AM, Hughes PF, Loisel DR, Hauck JS, Fu Y, Haystead TA, Huang J, Thiele DJ. Targeting therapy-resistant prostate cancer via a direct inhibitor of the human heat shock transcription factor 1. *Sci Transl Med.* 2020 Dec 16;12(574):eabb5647. doi: 10.1126/scitranslmed.abb5647. PMID: 33328331.

### In vivo study

1. Dong B, Jaeger AM, Hughes PF, Loisel DR, Hauck JS, Fu Y, Haystead TA, Huang J, Thiele DJ. Targeting therapy-resistant prostate cancer via a direct inhibitor of the human heat shock transcription factor 1. *Sci Transl Med.* 2020 Dec 16;12(574):eabb5647. doi: 10.1126/scitranslmed.abb5647. PMID: 33328331.

## 7. Bioactivity

### Biological target:

DTHIB is a direct and selective heat shock factor 1 (HSF1) inhibitor with a K<sub>d</sub> of 160 nM for DTHIB binding to the HSF1 DNA binding domain (DBD).

### In vitro activity

DTHIB robustly inhibited the HSF1 cancer gene signature and prostate cancer cell proliferation.

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Reference: Sci Transl Med. 2020 Dec 16;12(574):eabb5647. <https://pubmed.ncbi.nlm.nih.gov/33328331/>

## In vivo activity

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In addition, it (DTHIB) potently attenuated tumor progression in four therapy-resistant prostate cancer animal models, including an NEPC model, where it caused profound tumor regression.

Reference: Sci Transl Med. 2020 Dec 16;12(574):eabb5647. <https://pubmed.ncbi.nlm.nih.gov/33328331/>

*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.*