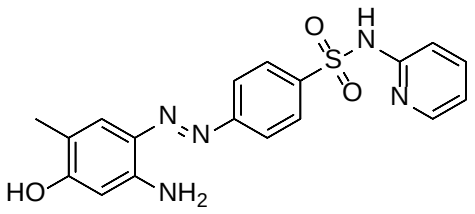
Product data sheet

MedKoo Cat#: 406976 Name: MS436 CAS: 1395084-25-9 Chemical Formula: $C_{18}H_{17}N_5O_3S$ Exact Mass: 383.1052 Molecular Weight: 383.426	
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:
MS436 is a BRD4 inhibitor. MS436, through a set of water-mediated interactions, exhibits low nanomolar affinity (estimated Ki of 30-50 nM). MS436 effectively inhibits BRD4 activity in NF-κB-directed production of nitric oxide and proinflammatory cytokine interleukin-6 in murine macrophages. MS436 represents a new class of bromodomain inhibitors and will facilitate further investigation of the biological functions of the two bromodomains of BRD4 in gene expression.

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	39.60	103.29

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.61 mL	13.04 mL	26.08 mL
5 mM	0.52 mL	2.61 mL	5.22 mL
10 mM	0.26 mL	1.30 mL	2.61 mL
50 mM	0.05 mL	0.26 mL	0.52 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. Yu X, Long Q, Shen S, Liu Z, Chandran J, Zhang J, Ding H, Zhang H, Cai D, Kim ES, Huang Y, Guo H. Screening of an epigenetic compound library identifies BRD4 as a potential antiviral target for hepatitis B virus covalently closed circular DNA transcription. Antiviral Res. 2023 Mar;211:105552. doi: 10.1016/j.antiviral.2023.105552. Epub 2023 Feb 1. PMID: 36737008.
2. Zhang G, Plotnikov AN, Rusinova E, Shen T, Morohashi K, Joshua J, Zeng L, Mujtaba S, Ohlmeyer M, Zhou MM. Structure-guided design of potent diazobenzene inhibitors for the BET bromodomains. J Med Chem. 2013 Nov 27;56(22):9251-64. doi: 10.1021/jm401334s. Epub 2013 Nov 11. PMID: 24144283; PMCID: PMC3894848.

In vivo study

TBD

7. Bioactivity
Biological target:

MS436 is a new class of bromodomain inhibitor, exhibits potent affinity of an estimated K_i=30-50 nM for the BRD4 BrD1.

In vitro activity

Product data sheet

Among the obtained hits, a bromodomain-containing protein 4 (BRD4) inhibitor MS436 exhibited marked inhibition of cccDNA transcription in both HBV stable cell line HepAD38 and HepG2-NTCP or primary human hepatocyte infection system under noncytotoxic concentrations. Chromatin immunoprecipitation (ChIP) assay demonstrated that MS436 dramatically reduced the enrichment of H3K27ac, an activating histone modification pattern, on cccDNA minichromosome.

Reference: Antiviral Res. 2023 Mar;211:105552. https://pubmed.ncbi.nlm.nih.gov/36737008/

In vivo activity

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.