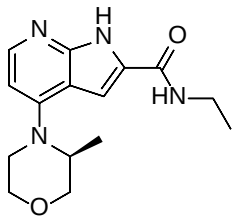
Product data sheet

MedKoo Cat#: 563699 Name: BAY-707 free base CAS#: 2109805-96-9 (free base) Chemical Formula: $C_{15}H_{20}N_4O_2$ Exact Mass: 288.1586 Molecular Weight: 288.35	
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:
BAY-707 is a substrate-competitive, highly potent and selective inhibitor of MTH1.

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	28.83	100.0
Ethanol	2.88	10.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.47 mL	17.34 mL	34.68 mL
5 mM	0.69 mL	3.47 mL	6.94 mL
10 mM	0.35 mL	1.73 mL	3.47 mL
50 mM	0.07 mL	0.35 mL	0.69 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. Ellermann M, Eheim A, Rahm F, Viklund J, Guenther J, Andersson M, Ericsson U, Forsblom R, Ginman T, Lindström J, Silvander C, Trésaugues L, Giese A, Bunse S, Neuhaus R, Weiske J, Quanz M, Glasauer A, Nowak-Reppel K, Bader B, Irlbacher H, Meyer H, Queisser N, Bauser M, Haegebarth A, Gorjánácz M. Novel Class of Potent and Cellularly Active Inhibitors Devalidates MTH1 as Broad-Spectrum Cancer Target. ACS Chem Biol. 2017 Aug 18;12(8):1986-1992. doi: 10.1021/acschembio.7b00370. Epub 2017 Jul 12. PMID: 28679043.

In vivo study

1. Ellermann M, Eheim A, Rahm F, Viklund J, Guenther J, Andersson M, Ericsson U, Forsblom R, Ginman T, Lindström J, Silvander C, Trésaugues L, Giese A, Bunse S, Neuhaus R, Weiske J, Quanz M, Glasauer A, Nowak-Reppel K, Bader B, Irlbacher H, Meyer H, Queisser N, Bauser M, Haegebarth A, Gorjánácz M. Novel Class of Potent and Cellularly Active Inhibitors Devalidates MTH1 as Broad-Spectrum Cancer Target. ACS Chem Biol. 2017 Aug 18;12(8):1986-1992. doi: 10.1021/acschembio.7b00370. Epub 2017 Jul 12. PMID: 28679043.

7. Bioactivity
Biological target: BAY-707 is an inhibitor of MTH1(NUDT1) with an IC50 of 2.3 nM.

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In vitro activity

The growth inhibitory effects of BAY-707 were investigated on several human cancer cell lines. Unexpectedly, despite BAY-707 being potent and cellularly active, no antiproliferative effects were observed with BAY-707 up to 30 μM (Figure 2C, Table S2). These results suggest that MTH1 is not required for cancer cell survival.

Reference: ACS Chem Biol. 2017 Aug 18;12(8):1986-1992. https://pubs.acs.org/doi/10.1021/acschembio.7b00370

In vivo activity

To investigate the efficacy of MTH1 inhibition in vivo, the antitumor efficacy of BAY-707 was evaluated. Two distinct tumor models were selected to explore potential antitumor activity of MTH1 inhibition: the syngeneic CT26 colon adenocarcinoma model (Figure 4C,D) and the NCI-H460 nonsmall cell lung cancer xenograft (Figure 4E,F). In the CT26 animal model, while radiation therapy provided the anticipated suppression of tumor growth, BAY-707 failed to provide significant antitumor activity in monotherapy or additive effects when combined with radiation treatment. Similar results were obtained testing the potent MTH1 inhibitor in the NCI-H460 model (Figure 4E,F). Once again, BAY-707 failed to provide in vivo antitumor activity as evidenced by no significant decrease in tumor volume or tumor weight.

Reference: ACS Chem Biol. 2017 Aug 18;12(8):1986-1992. https://pubs.acs.org/doi/10.1021/acschembio.7b00370