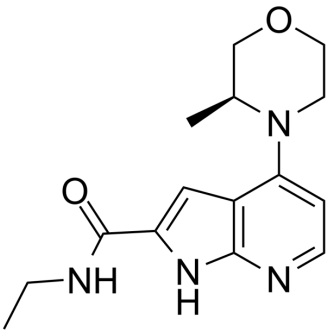
BAY-707

Cat. No.:	HY-112081
CAS No.:	2109805-96-9
Molecular Formula:	$C_{15}H_{20}N_4O_2$
Molecular Weight:	288.34
Target:	DNA/RNA Synthesis
Pathway:	Cell Cycle/DNA Damage
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	BAY-707 is a substrate-competitive, highly potent and selective inhibitor of MTH1(NUDT1) with an IC_{50} of 2.3 nM. BAY-707 has a good pharmacokinetic (PK) profile to other MTH1 compounds and is well-tolerated in mice, but shows a clear lack of in vitro or in vivo anticancer efficacy[1].
IC_{50} & Target	IC50:2.3 nM (MTH1/NUDT1)[1]
In Vitro	BAY-707 demonstrates a superior cellular target engagement with an EC_{50} of 7.6 nM, in agreement with its higher enzymatic potency (IC_{50}=2.3 nM)[1]. BAY-707 demonstrates a high cell permeability cell permeability in the Caco-2 assay with a efflux ratio of 288 nm/s[1]. BAY-707 shows an overall favorable physicochemical profile and promising in vitro pharmacokinetic properties with high metabolic stability in both human microsomes(0.29L/h/kg,F_{max}=78%) and rat hepatocytes (0.54L/h/kg,F_{max}=87%) [1]. BAY-707 (0-30 μM; 24 hours) has no antiproliferative effects in HMEC, HeLa and SW-480 cells[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Bay-077 (orally adminstation; 50-250 mg/kg; 2 weeks) exhibits superior biochemical potency, cellular target engagement, and a pharmacokinetic profile to other MTH1 tool compounds, But Bay-077 exerts no anticancer efficacy either in mono- or in combination therapies in CT26 and NCI-H460 mice model[1]. BAY-707 (orally adminstation; 50-250 mg/kg; 2 weeks) is well-tolerated in nude mice, after 7-days treatment, body weight loss does not exceed 10% [1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Ellermann M, et al. 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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