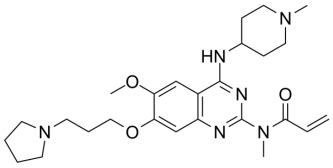
Antitumor agent-101

Cat. No.:	HY-155020
CAS No.:	2848632-52-8
Molecular Formula:	$C_{26}H_{38}N_6O_3$
Molecular Weight:	482.62
Target:	Histone Methyltransferase; GLP Receptor
Pathway:	Epigenetics; GPCR/G Protein
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description Antitumor agent-101 is a selective covalent inhibitor of lysine methyltransferases G9a/GLP, with IC_{50}s of 8.5 nM and 5.5 nM for G9a and GLP, respect
Antitumor agent-101 shows antitumor efficacy in the PANC-1 xenograft model[1].

IC_{50} & Target	G9a	GLP
	8.5 nM (IC_{50})	5.5 nM (IC_{50})

In Vitro

Antitumor agent-101 (Compound 27) (0-5 μM; 48 hours) significantly exhibits proliferation and colony formation of PANC-1 and MDA-MB-231 cells w
s of 2.68 and 2.88 μM, respectively[1].
Antitumor agent-101 (0-10 μM; 0-96 hours) effectively reduces H3K9me2 in PANC-1 and MDA-MB-231 cells in a concentration- and time-dependent m
[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	PANC-1 and MDA-MB-231 cells
Concentration:	0, 1.25, 2.5, 5 μM
Incubation Time:	48 hours
Result:	Ihibited proliferation of PANC-1 and MDA-MB-231 cells with IC_{50}s of 2.68 and 2.88 μM, respectively. Significantly suppressed the colony formation in MDA-MB-231 and PANC-1 cell lines at 2.5 μM.

Western Blot Analysis[1]

Cell Line:	PANC-1 and MDA-MB-231 cells
Concentration:	2.5, 5, 10 μM
Incubation Time:	4, 48, 72, or 96 hours
Result:	Effectively reduced H3K9me2 in PANC-1 and MDA-MB-231 cells in a concentration- and time-dependent manne Still significantly inhibited the levels of H3K9me2 in the cells treated with compound 27 were still significantly inhibited within 24h after Antitumor agent-101 was washed out, and the levels of H3K9me2 were recovered afte

In Vivo

Antitumor agent-101 (Compound 27) (2 mg/kg for i.p., 5 days a week) suppresses PANC-1 xenograft tumor growth by inhibiting the methyltransfera activity of G9a/GLP[1].

Antitumor agent-101 (2 mg/kg for p.o.) shows a C_{max} of 316 ng/mL, and mean residence time (MRT) of 0.61 hour[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	PANC-1 xenograft tumor models in male Balb/c nu/nu mice[1]
Dosage:	2 mg/kg
Administration:	Intraperitoneal injection (i.p.), 5 days a week (5 days on and 2 days off).
Result:	Exhibited potent antitumor activity with a tumor growth inhibition (TGI) rate of 52.2% with no obvious toxicity. Showed lower levels of H3K9me2 than the vehicle group.

Animal Model:	Male ICR Mice (Pharmacokinetic assay)[1]
Dosage:	2 mg/kg
Administration:	Intraperitoneal injection (i.p.)
Result:	Pharmacokinetic parameters for antitumor agent-101 (Compound 27) in rats [1]

Route	Dose (mg/kg)	C_{max} (ng/mL)	AUC_{0-t} (h•ng/mL)	$AUC_{0-\infty}$ (h•ng/mL)	MRT (h)
i.p.	2	316	208	214	0.61

REFERENCES

[1]. Feng Z, et.al. Structure-Based Design and Characterization of the Highly Potent and Selective Covalent Inhibitors Targeting the Lysine Methyltransferases G9a/ Med Chem. 2023 Jun 22;66(12):8086-8102.

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