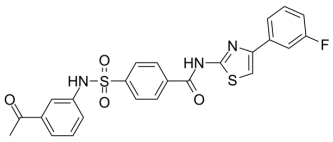
PHGDH-IN-3

Cat. No.:	HY-148570
CAS No.:	2893778-31-7
Molecular Formula:	$C_{24}H_{18}FN_3O_4S_2$
Molecular Weight:	495.55
Target:	Phosphoglycerate Dehydrogenase (PHGDH)
Pathway:	Metabolic Enzyme/Protease
Storage:	4°C, protect from light * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (201.80 mM; ultrasonic and warming and heat to 70°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0180 mL	10.0898 mL	20.1796 mL
	5 mM	0.4036 mL	2.0180 mL	4.0359 mL
	10 mM	0.2018 mL	1.0090 mL	2.0180 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (10.09 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PHGDH-IN-3 is an orally active phosphoglycerate dehydrogenase (PHGDH) inhibitor. PHGDH-IN-3 inhibits PHGDH with an IC_{50} value of 2.8 μM. PHGDH-IN-3 can be used for the research of cancer[1].

IC_{50} & Target

IC50: 2.8 μM (PHGDH)[1].
Kd: 2.33 μM (PHGDH)[1]

In Vitro

PHGDH-IN-3 (compound D8) has good enzymatic inhibitory activity with an IC_{50} value of 2.8 μM[1].
PHGDH-IN-3 has high binding affinity for the PHGDH protein with a K_d value of 2.33 μM[1].
PHGDH-IN-3 has sensitivity to the cell lines with the PHGDH gene amplification or overexpression[1].
PHGDH-IN-3 can restrict the de novo serine synthesis from glucose within MDA-MB-468 cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

PHGDH-IN-3 (compound D8) (p.o., i.v.; 1, 3 mg/kg) exhibits excellent in vivo pharmacokinetic properties[1].
PHGDH-IN-3 (i.p.; 12.5, 25, 50 mg/kg; once daily for consecutive 31 days) exertes evident antitumor efficacy in the PC9

xenograft mouse model[1].

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

Animal Model:	ICR mice[1]
Dosage:	1, 3 mg/kg
Administration:	Oral (p.o.) and intravenous (i.v.) administration
Result:	

PK parameters	i.v. (1 mg/kg)	p.o. (3 mg/kg)
AUC (h•ng/mL)	38,358 ± 14,768	94,386 ± 23,416
$T_{1/2}$(h)	4.94 ± 0.38	4.74 ± 0.30
T_{max} (h)		3.33 ± 1.15
CL_{obs}(mL/min/kg)	0.48 ± 0.23	
C_{max}(ng/mL)		8842 ± 1755
F (%)		82.0

Animal Model:	Balb/c nude mice[1]
Dosage:	12.5, 25, 50 mg/kg
Administration:	Intraperitoneal (i.p.); once daily for consecutive 31 days
Result:	Exhibited an in vivo anti-tumor effect and significantly delayed the tumor growth. Significantly abated the tumor weights of mice at 25 mg/ kg.

REFERENCES

[1]. Dingding Gao, et al. Discovery of Novel Drug-like PHGDH Inhibitors to Disrupt Serine Biosynthesis for Cancer Therapy. J Med Chem. 2023 Jan 12;66(1):285-305.

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