PKUMDL-WQ-2101

Cat. No.: HY-123269

CAS No.: 304481-72-9

Molecular Formula: $C_{14}H_{11}N_3O_6$

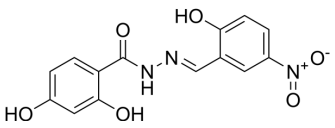
Molecular Weight: 317.25

Target: Phosphoglycerate Dehydrogenase (PHGDH)

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (394.01 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.1521 mL	15.7604 mL	31.5209 mL
	5 mM	0.6304 mL	3.1521 mL	6.3042 mL
	10 mM	0.3152 mL	1.5760 mL	3.1521 mL

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

BIOLOGICAL ACTIVITY

Description

PKUMDL-WQ-2101 is a non-NAD^+-competing allosteric phosphoglycerate dehydrogenase (PHGDH) inhibitor with an IC_{50} of 34.8 μM. PKUMDL-WQ-2101 exhibits antitumor activity[1].

IC_{50} & Target

IC50: 34.8 μM (PHGDH)[1]

In Vitro

PKUMDL-WQ-2101 (72 hours) shows dose-dependent suppression effects on the cell viability at micromolar concentrations, with good selectivity for PHGDH amplified breast cancer cell lines. The antitumor activities of PKUMDL-WQ-2101 in the two PHGDH amplified breast cancer cell lines (MDA-MB-468 and HCC70) are 7.70 μM and 10.8 μM, respectively[1].

PKUMDL-WQ-2101 (2.5-40 μM; 24 hours) causes cell cycle arrest in MDA-MB-468 cells[1].

PKUMDL-WQ-2101 (37 μM; 24 hours) decreases de novo serine synthesis and metabolism downstream of the serine synthesis pathway, with effects comparable to PHGDH genetic deletion[1].

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

Cell Viability Assay[1]

Cell Line:	MDA-MB-468 cells

Concentration:	2.5 μM, 5.0 μM, 20 μM and 40 μM
Incubation Time:	24 hours
Result:	Caused cell cycle arrest.

In Vivo

PKUMDL-WQ-2101 (5-20 mg/kg; i.p; daily; for 30 days) exhibits substantial inhibitory effects on MDA-MB-468 xenografts[1].

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

Animal Model:	NOD.CB17 Scid/J mice injected with MDA-MB-468 cells[1]
Dosage:	5 mg/kg, 10 mg/kg, 20 mg/kg
Administration:	i.p; daily; for 30 days
Result:	Exhibited substantial inhibitory effects on MDA-MB-468 xenografts.

REFERENCES

[1]. Qian Wang, et al. Rational Design of Selective Allosteric Inhibitors of PHGDH and Serine Synthesis with Anti-tumor Activity. Cell Chem Biol. 2017 Jan 19;24(1):55-65.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA