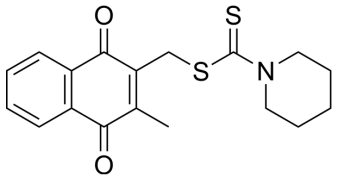
PKM2-IN-1

Cat. No.:	HY-103617
CAS No.:	94164-88-2
Molecular Formula:	$C_{18}H_{19}NO_2S_2$
Molecular Weight:	345.48
Target:	Pyruvate Kinase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 1 year -20°C 6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : 10 mg/mL (28.95 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8945 mL	14.4726 mL	28.9452 mL
	5 mM	0.5789 mL	2.8945 mL	5.7890 mL
	10 mM	0.2895 mL	1.4473 mL	2.8945 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 8 mg/mL (23.16 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 8 mg/mL (23.16 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 8 mg/mL (23.16 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PKM2-IN-1 (compound 3k) is a pyruvate kinase M2 (PKM2) inhibitor with an IC_{50} of 2.95 μM[1].

IC_{50} & Target

IC50: 2.95 μM (PKM2)[1]

In Vitro

PKM2-IN-1 (compound 3k) is a pyruvate kinase M2 (PKM2) inhibitor with an IC_{50} of 2.95±0.53 μM. Results show that most of the tested compounds exhibit some degree of PKM2 inhibition and some compounds, such as PKM2-IN-1 (compound 3k) and 6d, display more potent activity than the positive control shikonin. The representative compounds PKM2-IN-1, 6d

display dose-dependent inhibition of PKM2 with less inhibition of PKM1 and PKL like shikonin. Among all tested compounds, the most potent compounds are 3a, PKM2-IN-1 and 3r, which exhibit IC_{50} values against HCT116 and Hela cells ranging from 0.39 to 0.41 μM, 0.18 to 0.29 μM and 0.18 to 0.38 μM, respectively[1].

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

PROTOCOL

Cell Assay [1]

Cell lines (HCT116, Hela, H1299, BEAS-2B) are cultured in RPMI 1640 containing 9% fetal bovine serum (FBS) at 37°C in 5% CO_2. Cell viability is detected with the MTS assay according to the manufacturer's instructions. Briefly, 5000 cells in per well are plated in 96-well plates. After incubated for 12 h, the cells are treated with different concentration of tested compound (including PKM2-IN-1) or DMSO (as negative control) for 48 h. Then 20 μL MTS is added in per well and incubated at 37°C for 3 h. Absorbance of each well is determined by a microplate reader at a 490 nm wavelength. The IC_{50} values are calculated using Prism Graphpad software of the triplicate experiment[1].

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

CUSTOMER VALIDATION

- Sci Adv. 2022 Sep 23;8(38):eabo0987.
- Redox Biol. 2024 Mar 4:71:103112.
- EBioMedicine. 2020 Apr;54:102722.
- Cell Rep. 2022 Mar 8;38(10):110468.
- J Pathol. 2022 Apr;256(4):414-426.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Ning X, et al. Discovery of novel naphthoquinone derivatives as inhibitors of the tumor cell specific M2 isoform of pyruvate kinase. Eur J Med Chem. 2017 Sep 29;138:343-352.

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