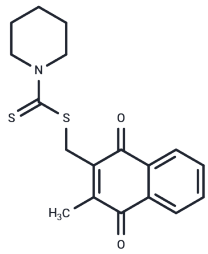
Data Sheet (Cat.No.T4170)

TargetMol

PKM2-IN-1

Chemical Properties



CAS No. : 94164-88-2

Formula: C18H19NO2S2

Molecular Weight: 345.48

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	PKM2-IN-1 (compound 3k) exhibits inhibitory activity against PKM2 with an IC50 of 2.95 μM, while the IC50 for PKM1 is 4-5 times higher.
Targets(IC50)	PKM
In vitro	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 IC50 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.
Cell Research	Cell lines (HCT116, Hela, H1299, BEAS-2B) are cultured in RPMI 1640 containing 9% fetal bovine serum (FBS) at 37°C in 5% CO2. 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. The absorbance of each well is determined by a microplate reader at a 490 nm wavelength. The IC50 values are calculated using Prism Graphpad software of the triplicate experiment.

Solubility Information

Solubility	DMSO: 2.11 mg/mL (6.11 mM),Sonication is recommended. Ethanol: < 1 mg/mL (insoluble or slightly soluble), H2O: < 1 mg/mL (insoluble or slightly soluble), (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.8945 mL	14.4726 mL	28.9452 mL
5 mM	0.5789 mL	2.8945 mL	5.789 mL
10 mM	0.2895 mL	1.4473 mL	2.8945 mL
50 mM	0.0579 mL	0.2895 mL	0.5789 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.
Deng H, Qian X, Zhang Y, et al.Metformin Increases the Response of Cholangiocarcinoma Cells to Gemcitabine by Suppressing Pyruvate Kinase M2 to Activate Mitochondrial Apoptosis.Digestive Diseases and Sciences.2024: 1-15.