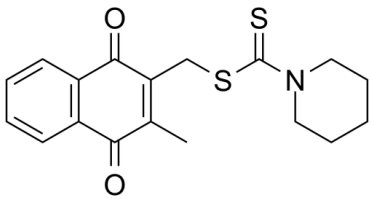
Data Sheet

Product Name:	PKM2-IN-1
Cat. No.:	CS-8094
CAS No.:	94164-88-2
Molecular Formula:	C18H19NO2S2
Molecular Weight:	345.48
Target:	Pyruvate Kinase
Pathway:	Metabolic Enzyme/Protease
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 5.56 mg/mL (16.09 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

PKM2-IN-1 is a **pyruvate kinase M2** (**PKM2**) inhibitor with an **IC_{50}** of 2.95 μM. IC50 & Target: IC50: 2.95 μM (PKM2)[1] **In Vitro:** PKM2-IN-1 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].

PROTOCOL (Extracted from published papers and Only for reference)

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].

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.

CAIndexNames:

1-Piperidinecarbodithioic acid, (1,4-dihydro-3-methyl-1,4-dioxo-2-naphthalenyl)methyl ester

SMILES:

S=C(N1CCCCC1)SCC(C2=O)=C(C)C(C3=C2C=CC=C3)=O

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

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