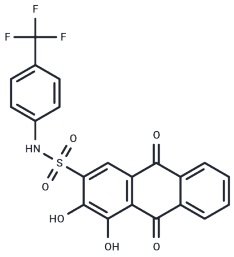
Data Sheet (Cat.No.T16517)

TargetMol

PGMI-004A

Chemical Properties



CAS No. : 1313738-90-7

Formula: C21H12F3NO6S

Molecular Weight: 463.38

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	PGMI-004A is an effective inhibitor of phosphoglycerate mutase 1 (IC50: 13.1 μM).
Targets(IC50)	Phosphatase
In vitro	PGMI-004A inhibits PGAM1 with an IC50 of approximately 13.1 μM and the Kd value of the PGMI-004A-PGAM1 interaction is determined to be 7.2±0.7 μM from the fluorescence-based binding assay. PGMI-004A treatment induces decreased cell proliferation of diverse human cancer and leukemia cells, but not control human dermal fibroblasts (HDF), human foreskin fibroblasts (HFF), human HaCaT keratinocyte cells and human melanocyte PIG1 cells, suggesting minimal non-specific toxicity of PGMI-004A in normal, proliferating human cells. PGMI-004A may allosterically modulate the enzyme activity of PGAM1. The Ki value is determined to be 3.91±2.50 μM using a Dixon plot analysis. The Kd value for protein-ligand interaction is calculated to be 9.4±2.0 μM. PGMI-004A (20 μM) treatment, causes significantly reduced lactate production that is rescued by methyl-2-PG treatment but has no significant effect on intracellular ATP levels. Inhibition of PGAM1 activity by PGMI-004A (20 μM) treatment results in decreased 2-PG and increased 3-PG levels in H1299 cells, which could be rescued by treatment with methyl-2-PG. PGMI-004A (20 μM) treatment results in decreased oxidative PPP flux and NADPH/NADP+ratio, as well as reduced biosynthesis of lipids and RNA, and cell proliferation in H1299 cells [1].
In vivo	Treatment with PGMI-004A significantly reduces tumor growth and size in mice when compared to those treated with a vehicle control. It effectively inhibits PGAM1 enzyme activity within tumors of nude mice bearing xenografts. The xenograft model is established by injecting H1299 cells into nude mice, and after six days, the mice are segregated into two groups (n=8/group). They are subsequently treated with either PGMI-004A (100mg/kg/day) or a vehicle for 21 days [1].

Solubility Information

Solubility	DMSO: 125 mg/mL (269.76 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (7.12 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1581 mL	10.7903 mL	21.5806 mL
5 mM	0.4316 mL	2.1581 mL	4.3161 mL
10 mM	0.2158 mL	1.079 mL	2.1581 mL
50 mM	0.0432 mL	0.2158 mL	0.4316 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

Hitosugi T, et al. Phosphoglycerate mutase 1 coordinates glycolysis and biosynthesis to promote tumor growth. Cancer Cell. 2012 Nov 13;22(5):585-600.