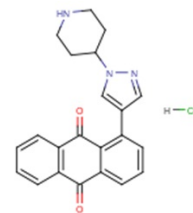


PDK4-IN-1 hydrochloride

Chemical Properties

CAS No.:	2310262-11-2
Formula:	C ₂₂ H ₂₀ ClN ₃ O ₂
Molecular Weight:	393.87
Appearance:	N/A
Storage:	0-4°C for short term (days to weeks), or -20°C for long term (months).



Biological Description

Description	PDK4-IN-1 hydrochloride is an anthraquinone derivative and a potent and orally active inhibitor of pyruvate dehydrogenase kinase 4 (PDK4)(IC ₅₀ value of 84 nM)
Targets(IC ₅₀)	Pyruvate dehydrogenase kinase 4 (PDK4): 84 nM
In vitro	PDK4-IN-1 hydrochloride treatment significantly impedes the proliferation of human colon cancer cell lines, HCT116 and RKO. The colony formation efficiency in HCT116 and RKO cells is significantly reduced after treatment of PDK4-IN-1[1]. PDK4-IN-1 (Compound 8c; 10-50 μM; 24 hours; HCT116 and RKO cells) treatment dose-dependently increased apoptosis. PDK4-IN-1 decreases the expression of BCL-xL and increases the expression of BAX. Cleavage of PARP1 and caspase 3 are increased by PDK4-IN-1[1].
In vivo	PDK4-IN-1 (C57BL/6J mice) treatment significantly improves glucose tolerance[1]. Pre-incubation with PDK4-IN-1 (compound 8c) dose-dependently inhibits the release of β-hexosaminidase from IgE/antigen-activated BMDCs,

Solubility Information

Solubility	DMSO: 125 mg/mL (317.36 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.539 mL	12.695 mL	25.389 mL
5 mM	0.508 mL	2.539 mL	5.078 mL
10 mM	0.254 mL	1.269 mL	2.539 mL
50 mM	0.051 mL	0.254 mL	0.508 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 °C for 6 months; - 20 °C for 1 month. Please use it as soon as possible.

Reference

1. Lee D, et al. Discovery of Novel Pyruvate Dehydrogenase Kinase 4 Inhibitors for Potential Oral Treatment of Metabolic Diseases. J Med Chem. 2019 Jan 24;62(2):575-588.

Inhibitors · Natural Compounds · Compound Libraries

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