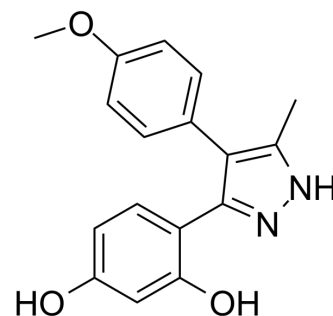


M77976

Cat. No.:	HY-114702		
CAS No.:	394237-61-7		
Molecular Formula:	C ₁₇ H ₁₆ N ₂ O ₃		
Molecular Weight:	296.32		
Target:	PDHK		
Pathway:	Metabolic Enzyme/Protease		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro	DMSO : 250 mg/mL (843.68 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	3.3747 mL	16.8736 mL	33.7473 mL
		5 mM	0.6749 mL	3.3747 mL	6.7495 mL
10 mM		0.3375 mL	1.6874 mL	3.3747 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (7.02 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.08 mg/mL (7.02 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (7.02 mM); Clear solution 				

BIOLOGICAL ACTIVITY

Description	M77976 is a specific ATP-competitive inhibitor of PDK4 (pyruvate dehydrogenase kinase isoforms 4), with an IC ₅₀ of 648 μM. M77976 is potential for the research of obesity and diabetes ^[1] .
IC₅₀ & Target	IC ₅₀ : 648 μM (PDK4) ^[1]
In Vitro	M77976 binds to the ATP-binding pocket of PDK4 and causes local conformational changes with complete disordering of the ATP lid ^[1] .

M77976 makes hydrophobic interactions with the side chains of Asn258, Ala262, Val298, Leu306 and Thr358 of PDK4^[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Kukimoto-Niino M, et al. Inhibitor-bound structures of human pyruvate dehydrogenase kinase 4. Acta Crystallogr D Biol Crystallogr. 2011 Sep;67(Pt 9):763-73.

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

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