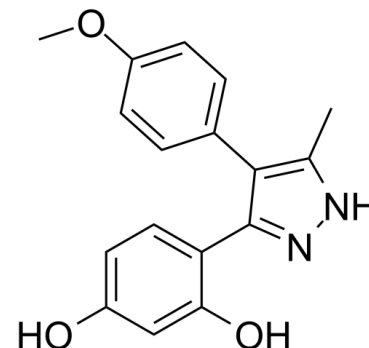


Data Sheet

Product Name:	M77976
Cat. No.:	CS-0064130
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
Solubility:	DMSO : 250 mg/mL (843.68 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

M77976 is a specific ATP-competitive inhibitor of **PDK4 (pyruvate dehydrogenase kinase isoforms 4)**, with an **IC₅₀** of 648 μM. M77976 is potential for the research of obesity and diabetes^[1]. **IC₅₀ & Target:** IC₅₀: 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].

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.

CAIndexNames:

1,3-Benzenediol, 4-[4-(4-methoxyphenyl)-5-methyl-1H-pyrazol-3-yl]-

SMILES:

COC1=CC=C(C=C1)C2=C(NN=C2C3=CC=C(C=C3O)O)C

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

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