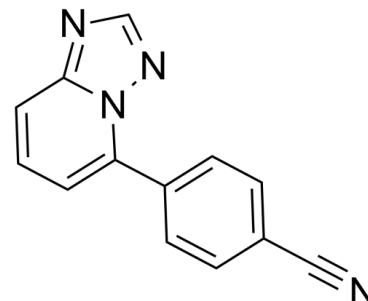


Data Sheet

Product Name:	PHD-1-IN-1
Cat. No.:	CS-0127937
CAS No.:	2009343-14-8
Molecular Formula:	C ₁₃ H ₈ N ₄
Molecular Weight:	220.23
Target:	HIF/HIF Prolyl-Hydroxylase
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : 195 mg/mL (885.44 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

PHD-1-IN-1 is an orally active and potent **HIF prolylhydroxylase domain-1 (PHD-1)** inhibitor with an **IC₅₀** of 0.034 μM. PHD-1-IN-1 has a unique monodentate binding interaction with the active site Fe²⁺ ion and induces the formation of an “Arg367-out” pocket^[1].
IC₅₀ & Target: IC₅₀: 0.034 μM (PHD-1)^[1] **In Vivo:** PHD-1-IN-1 (compound 17; 3 mg/kg of p.o. or 0.5 mg/kg of i.v.) has a C_{max} of 0.8 μM, a AUC of 176 ng•h/mL, K_{p,uu} of 1.11 and B/P of 0.95^[1].

References:

[1]. Ahmed S, et al. 1,2,4-Triazolo-[1,5-a]pyridine HIF Prolylhydroxylase Domain-1 (PHD-1) Inhibitors With a Novel Monodentate Binding Interaction. J Med Chem. 2017 Jul 13;60(13):5663-5672.

CAIndexNames:

Benzonitrile, 4-[1,2,4]triazolo[1,5-a]pyridin-5-yl-

SMILES:

N#CC1=CC=C(C2=CC=CC3=NC=NN23)C=C1

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

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