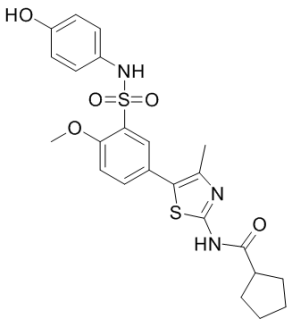
PI4KIIIbeta-IN-9

Cat. No.:	HY-19798
CAS No.:	1429624-84-9
Molecular Formula:	$C_{23}H_{25}N_3O_5S_2$
Molecular Weight:	487.59
Target:	PI4K; PI3K
Pathway:	PI3K/Akt/mTOR
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (205.09 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0509 mL	10.2545 mL	20.5090 mL
	5 mM	0.4102 mL	2.0509 mL	4.1018 mL
	10 mM	0.2051 mL	1.0255 mL	2.0509 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.13 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.13 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.13 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PI4KIIIbeta-IN-9 is a potent PI4KIIIβ inhibitor with an IC_{50} of 7 nM. PI4KIIIbeta-IN-9 also inhibits PI3Kδ and PI3Kγ with IC_{50}s of 152 nM and 1046 nM, respectively.

IC_{50} & Target

PI4KIIIβ 7 nM (IC_{50})	PI4KIIIα 2.6 μM (IC_{50})	PI3Kδ 152 nM (IC_{50})	PI3Kγ 1046 nM (IC_{50})
PI3Kα 2 μM (IC_{50})	PI3KC2γ 1 μM (IC_{50})		

In Vitro	PI4KIIIbeta-IN-9 (Compound 9) shows weak inhibition of PI3KC2γ (IC_{50} ~1 μM), PI3Kα (~2 μM), and PI4KIIIα (~2.6 μM) and <50% inhibition at concentrations up to 20 μM for PI4K2α, PI4K2β, and PI3Kβ. PI4KIIIbeta-IN-9 (Compound 9) forms a crescent shape that conforms to the active site of PI4KIIIβ. This molecule makes extensive contacts with PI4KIIIβ[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Rutaganira FU, et al. Design and Structural Characterization of Potent and Selective Inhibitors of Phosphatidylinositol 4 Kinase IIIβ. J Med Chem. 2016 Mar 10;59(5):1830-9.

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