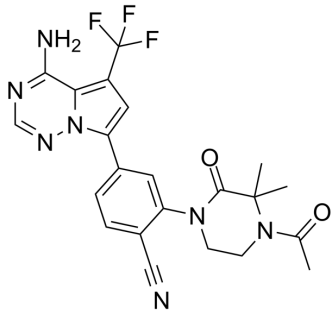
PI3Kδ-IN-1



Cat. No.:	HY-101921
CAS No.:	1911564-39-0
Molecular Formula:	$C_{22}H_{20}F_3N_7O_2$
Molecular Weight:	471.44
Target:	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 : 62.5 mg/mL (132.57 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1212 mL	10.6058 mL	21.2116 mL
	5 mM	0.4242 mL	2.1212 mL	4.2423 mL
	10 mM	0.2121 mL	1.0606 mL	2.1212 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: 2.08 mg/mL (4.41 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.41 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PI3Kδ-IN-1 is a potent, selective, and efficacious PI3Kδ inhibitor with an IC_{50} of 1.7 nM.

IC_{50} & Target

IC50: 1.7 nM (PI3Kδ)[1]

In Vitro

PI3Kδ-IN-1 (compound 52) shows >100-fold selectivity over the other PI3K isoforms. Kinome selectivity is also excellent with >660-fold selectivity over MNK1 and others in HTRF assays. Importantly, PI3Kδ-IN-1 has an improved human/rodent in vitro stability correlation and a good permeability profile[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

PI3Kδ-IN-1 (2, 5 mg/kg, orally b.i.d. for 42 days) shows greater than 50% suppression of paw swelling in mice. PI3Kδ-IN-1 has

an EC_{50} of 10 nM at 24 h (ED_{50} of -1.25 mg/kg) in mice[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male DBA/1 mice (20–25g)[1]
Dosage:	0.5, 2, 5 mg/kg
Administration:	Oral b.i.d. for 42 days,
Result:	A dose dependent reduction of the clinical score was observed. Doses of 2 and 5 mg/kg showed greater than 50% suppression of paw swelling[1].

REFERENCES

[1]. Liu Q, et al. Identification of a Potent, Selective, and Efficacious Phosphatidylinositol 3-Kinase δ (PI3Kδ) Inhibitor for the Treatment of Immunological Disorders. J Med Chem. 2017 Jun 22;60(12):5193-5208.

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