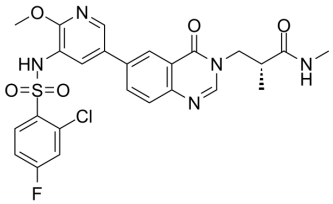
PI3Kα-IN-4

Cat. No.:	HY-131345
CAS No.:	2322293-83-2
Molecular Formula:	$C_{25}H_{23}ClFN_5O_5S$
Molecular Weight:	560
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 : 100 mg/mL (178.57 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.7857 mL	8.9286 mL	17.8571 mL
5 mM	0.3571 mL	1.7857 mL	3.5714 mL
10 mM	0.1786 mL	0.8929 mL	1.7857 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 (4.46 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.46 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.46 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PI3Kα-IN-4 is a potent, selective and orally active inhibitor of PI3Kα, with an IC_{50} of 1.8 nM. PI3Kα-IN-4 has antitumor activity [1].

IC_{50} & Target

PI3Kα
1.8 nM (IC_{50})

In Vitro

PI3Kα-IN-4 (compound 10) inhibits PI3Kα, β, δ, and γ, with IC_{50}s of 1.8, 271.0, 13.9, and 13.8 nM, respectively in kinase assays

	[1]. PI3Kα-IN-4 inhibits PI3Kα, β, δ, and γ, with IC_{50}s of 12.1,1393, 183, and >10000 nM, respectively in cell based assays[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	PI3Kα-IN-4 (compound 10) (30 mg/kg; p.o. once daily for 21 d) achieves the best efficacy, which could inhibit tumor growth by 73.0% in mice[1]. PI3Kα-IN-4 (15-40 mg/kg; p.o. once daily for 30 d) dose dependently suppresses tumor growth by 62.5% (15 mg/kg), 86.0% (30 mg/kg) and 90.7% (40 mg/kg), respectively in mice[1]. PI3Kα-IN-4 (15-40 mg/kg; p.o. once daily; 1-4 h) inhibits the phosphorylation of Akt in a dose- and time-dependent manner in vivo[1]. PI3Kα-IN-4 shows high C_{max} (mouse 22167, rat 2327 nM) and good bioavailability (mouse 59.4%, rat 46.9%) following oral administration (mouse 10, rat 3 mg/kg)[1]. PI3Kα-IN-4 shows $t_{1/2}$ (mouse 0.99, rat 1.22 h) and low plasma clearance (mouse 4.16, rat 5.28 mL/min/kg) following intravenous injection (mouse 1, rat 1 mg/kg)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	BT-474 subcutaneous xenograft mice[1]
Dosage:	30 mg/kg
Administration:	P.o. once daily for 21 days
Result:	Inhibited tumor growth by 73.0% and could be tolerated.

REFERENCES

[1]. Dong J, et, al. Discovery of 3-Quinazolin-4(3 H)-on-3-yl-2, N-dimethylpropanamides as Orally Active and Selective PI3Kα Inhibitors. ACS Med Chem Lett. 2020 Jun 10; 11(7): 1463-1469.

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

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