(S)-PI3Kα-IN-4

Cat. No.: HY-131345A

CAS No.: 2322293-84-3

Molecular Formula: $C_{25}H_{23}ClFN_5O_5S$

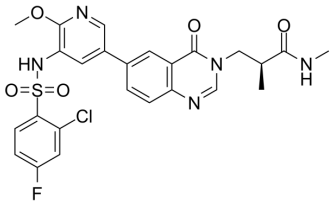
Molecular Weight: 560

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

(S)-PI3Kα-IN-4 is a potent inhibitor of PI3Kα, with an IC_{50} of 2.3 nM. (S)-PI3Kα-IN-4 shows 38.3-, 4.25-, and 4.93-fold selectivity for PI3Kα over PI3Kβ, PI3Kδ, and PI3Kγ, respectively. (S)-PI3Kα-IN-4 can be used for the research of cancer[1].

IC_{50} & Target

PI3Kα
2.3 nM (IC_{50})

In Vitro

(S)-PI3Kα-IN-4 (compound 11) is a quinazolin-4(3H)-one derivative with 2-substituted-N-methylpropanamide substitution[1].

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

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.

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