PI3K/mTOR Inhibitor-13 sodium

Cat. No.: HY-153120A

CAS No.: 2361009-23-4

Molecular Formula: $C_{20}H_{13}F_2N_5NaO_3S$

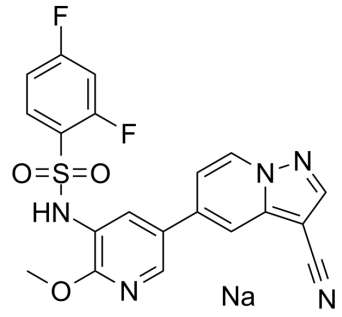
Molecular Weight: 464.4

Target: PI3K; mTOR

Pathway: PI3K/Akt/mTOR

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (215.33 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1533 mL	10.7666 mL	21.5332 mL
	5 mM	0.4307 mL	2.1533 mL	4.3066 mL
	10 mM	0.2153 mL	1.0767 mL	2.1533 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 (5.38 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.38 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.38 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

PI3K/mTOR Inhibitor-13 sodium is an orally active dual inhibitor of phosphoinositol 3-kinase (PI3K) and mTOR kinase. PI3K/mTOR Inhibitor-13 sodium has potential applications in sexual diseases, solid tumor and idiopathic pulmonary fibrosis (IPF)[1][2].

In Vitro

PI3K/mTOR Inhibitor-13 sodium (Compound A) (0-2 μM; 48 h) inhibits the proliferation of HFL1 cells with dose-dependent manner[1].

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

Cell Proliferation Assay[1]

Cell Line:	HFL1 cells.
Concentration:	0, 0.03125, 0.0125, 0.025, 0.05, 0.0625, 0.1, 0.125, 0.2, 0.25, 0.4, 0.5, 1 and 2 μM.
Incubation Time:	48 h.
Result:	Showed inhibitory for HFL1 cells.

Western Blot Analysis[1]

Cell Line:	HFL1 cells.
Concentration:	200 nM.
Incubation Time:	48 h.
Result:	Increased the expression of α-SMA/Tubulin.

In Vivo

Pharmacokinetic (PK) parameters of PI3K/mTOR Inhibitor-13 sodium[2]

Species	Administration manner	Dose (mg/kg)	$T_{1/2}$ (h)	AUC_{last} (ng•h/mL)	Cl/F (L/h/kg)	V_{ss} (L/kg)	F (%)
Rat	Intravenous injection	2	2.77	7069	0.29	0.85	94.75
Mice	Intravenous injection	1	5.45	57059	0.02	0.13	79.3
Dog	Intravenous injection	1	0.67	3672	0.27	0.23	108.5
Monkey	Intravenous injection	1	9.70	5978	0.16	0.92	59.8

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

REFERENCES

[1]. Cao S, et al. Pharmaceutical combination or pharmaceutical composition for treatment of fibrotic diseases. World Intellectual Property Organization. WO2020078445.

[2]. Xi N, et al. Aromatic heterocyclic compounds, pharmaceutical composition containing compounds and application of pharmaceutical composition.China.CN103965199.

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