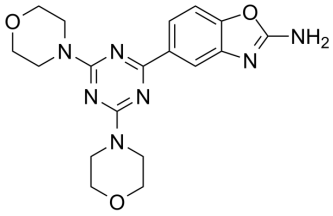
PI3Kα-IN-9

Cat. No.:	HY-150618
CAS No.:	2715287-67-3
Molecular Formula:	$C_{18}H_{21}N_7O_3$
Molecular Weight:	383.4
Target:	PI3K; Apoptosis
Pathway:	PI3K/Akt/mTOR; Apoptosis
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 (260.82 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6082 mL	13.0412 mL	26.0824 mL
	5 mM	0.5216 mL	2.6082 mL	5.2165 mL
	10 mM	0.2608 mL	1.3041 mL	2.6082 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 (6.52 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 (6.52 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (6.52 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

PI3Kα-IN-9 (compound 27) is a selective, long-acting and oral active PI3Kα inhibitor with IC_{50} values of 4.4, 128, 146 and 153 nM for PI3Kα, PI3Kγ, PI3Kδ and PI3Kβ, respectively. PI3Kα-IN-9 has antiproliferative activity and induces apoptosis. PI3Kα-IN-9 can be used for cancer research[1].

IC_{50} & Target	PI3Kα	PI3Kγ	PI3Kδ	PI3Kβ
	4.4 nM (IC_{50})	128 nM (IC_{50})	146 nM (IC_{50})	153 nM (IC_{50})

In Vitro

PI3Kα-IN-9 (compound 27) (0-8 μM; 72 hours; cancer cell lines) has antiproliferative activity and induces apoptosis[1].
PI3Kα-IN-9 (compound 27) (0-8 μM; MGC-803 cells) down-regulates the expression of PI3Kα protein, the proteins of PI3K downstream, p-AKT and p-P70S6 K[1].

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

Cell Viability Assay[1]

Cell Line:	MGC-803 (gastric cancer), SKOV-3 (ovarian cancer), PC-3(prostate cancer), MCF-7 (breast cancer), MDA-MB-231 (triple-negative breast cancer), HepG2 (liver cancer), RPMI8226 (multiple myeloma), K562 (chronic myeloid leukemia), U251 (glioma) and MOLT-4 (acute lymphoblastic leukemia) cell lines
Concentration:	0-2 μM
Incubation Time:	72 hours
Result:	Inhibited the growth of a variety of cancer cells with IC_{50} values ranging from 0.43 to 1.33 μM.

Apoptosis Analysis[1]

Cell Line:	MGC-803 cells
Concentration:	0, 2, 4 and 8 μM
Incubation Time:	36 hours
Result:	Increased the percentage of apoptotic cells from 12.07 to 61.69% in a dose-dependent manner.

In Vivo

PI3Kα-IN-9 (compound 27) (1-10 mg/kg; p.o. and i.v.; for 24 hours; male Sprague-Dawley rat) has favorable stability ($T_{1/2}$>10 h) and high bioavailability (130%)[1].
PI3Kα-IN-9 (compound 27) (30 mg/kg; p.o.; daily, for 3 weeks; male BALB/c nude mice) has antitumor activity and low cytotoxicity[1].

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

Animal Model:	Male Sprague-Dawley rat[1]
Dosage:	1 and 10 mg/kg
Administration:	Oral administration and intravenous injection; for 24 hours (Pharmacokinetic Analysis)
Result:	

parameters	IV	PO
dose (mg/kg)	1	10
$T_{1/2}$ (h)	6.29	10
T_{max} (h)	0.003	9.33
C_{max} (ng/mL)	454.7	2256.7

AUC_{0-t} (ng·h/mL)	2237	36697
$AUC_{0-\infty}$ (ng·h/mL)	2922.4	38114.3
CL (mL/h/kg)	343	
F %		130.4

Animal Model:	Male BALB/c nude mice[1]
Dosage:	30 mg/kg
Administration:	Oral administration; daily, for 3 weeks
Result:	Inhibited tumor growth with a tumor growth inhibition (TGI) rate of 41.5%.

REFERENCES

[1]. Hou Y, et, al. Discovery of Novel Phosphoinositide-3-Kinase α Inhibitors with High Selectivity, Excellent Bioavailability, and Long-Acting Efficacy for Gastric Cancer. J Med Chem. 2022 Jul 14.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA