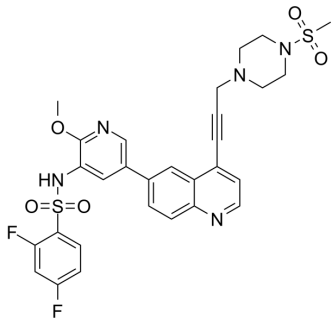
NSC781406

Cat. No.:	HY-100470
CAS No.:	1676893-24-5
Molecular Formula:	$C_{29}H_{27}F_2N_5O_5S_2$
Molecular Weight:	627.68
Target:	PI3K; mTOR
Pathway:	PI3K/Akt/mTOR
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 150 mg/mL (238.98 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.5932 mL	7.9658 mL	15.9317 mL
5 mM	0.3186 mL	1.5932 mL	3.1863 mL
10 mM	0.1593 mL	0.7966 mL	1.5932 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: 3.75 mg/mL (5.97 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3.75 mg/mL (5.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NSC781406 is a highly potent PI3K and mTOR inhibitor with an IC_{50} of 2 nM for PI3Kα.

IC_{50} & Target

PI3Kα 2 nM (IC_{50})	PI3Kγ 2.7 nM (IC_{50})	PI3Kβ 9.4 nM (IC_{50})	PI3Kδ 14 nM (IC_{50})
mTOR 5.4 nM (IC_{50})			

In Vitro

NSC781406 demonstrates potent PI3K inhibition (PI3Kα IC_{50}=2.0 nM) that translates into BEL-7404 cells proliferation inhibition (IC_{50}=20 nM). NSC781406 displays reasonable liver microsome stability. NSC781406 demonstrates cytotoxic

	activities against leukemia, non-small cell, lung cancer, colon cancer, central nervous system cancer, melanoma, ovarian cancer, renal cancer, prostate cancer, and breast cancer. It is potent against 60 cancer cell lines with a mean GI_{50} value of 65 nM, and with a GI50 value less than 10 nM against four cancer cell lines[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	In the xenograft models, treatment with 30 mg/kg of NSC781406 results in statistically significant antitumor activity, with a mean reduction in relative tumor volume ratio of 52%. Sorafenib displays an inhibition ratio of 44% at 50 mg/kg. NSC781406 is well tolerated at 30 mg/kg, with no observed mortality or significant reduction of body weight[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	IC_{50} values for inhibition of the PI3K is measured. PI-103 is used as the reference compound. The compounds (NSC781406) are tested in duplicate for 10 concentrations, 100 nM or 500 nM as the top concentration. All reagents are diluted in kinase buffer.Three-fold, ten-point serial compound (NSC781406) dilutions are performed in kinase buffer[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Cell Assay [1]	Cytotoxic effects are tested in the human lung adenocarcinoma cells A549, human colon cancer cells HCT-116, human breast cancer cells MDA-MB-231 and human hepatocellular carcinoma cells BEL-7404. These four tumor cells are diluted to a density of 40,000–50,000 cells/mL in logarithmic phase. After the cells are treated with compounds (NSC781406) for 72 h, MTT solution (5 mg/mL, 20 μL) is added another 4h at 37°C. IC_{50} values are determined by a nonlinear regression analysis[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Mice: NSC781406 is orally administered once a day 30 mg/kg for 14 consecutive days or with sorafenib at 50 mg/kg. The relative tumor volume to vehicle-treated control mice is monitored[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Mol Med. 2024 Feb 21;30(1):28.
- Front Pharmacol. 2020 Nov 11;11:580407.

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REFERENCES

[1]. Chen Y, et al. Discovery of benzenesulfonamide derivatives as potent PI3K/mTOR dual inhibitors with in vivo efficacies against hepatocellular carcinoma. Bioorg Med Chem. 2016 Mar 1;24(5):957-66.

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