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产品名称：NSC781406
产品别名：NSC781406

生物活性：

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

IC_{50} & Target	PI3Kα	PI3Kγ	PI3Kβ	PI3Kδ	mTOR
	2 nM (IC_{50})	2.7 nM (IC_{50})	9.4 nM (IC_{50})	14 nM (IC_{50})	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].
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].

Solvent&Solubility

In Vitro:

DMSO : ≥ 150 mg/mL (238.98 mM)

* "≥" means soluble, but saturation unknown.

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

*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 6 months; -20°C, 1 month。-80°C 储存时，请在 6 个月内使用，-20°C 储存时，请在 1 个月内使用。

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.

实验参考：

Cell Assay	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].
Animal Administration	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].

Kinase Assay	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].
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.