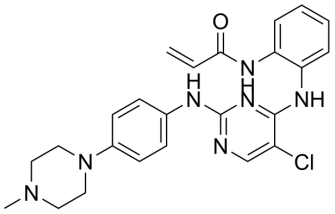
SM1-71

Cat. No.:	HY-136848
CAS No.:	2088179-99-9
Molecular Formula:	$C_{24}H_{26}ClN_7O$
Molecular Weight:	463.96
Target:	MAP3K; Src; FGFR; Ribosomal S6 Kinase (RSK); LIM Kinase (LIMK)
Pathway:	MAPK/ERK Pathway; Protein Tyrosine Kinase/RTK; Cell Cycle/DNA Damage
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 : 125 mg/mL (269.42 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1554 mL	10.7768 mL	21.5536 mL
	5 mM	0.4311 mL	2.1554 mL	4.3107 mL
	10 mM	0.2155 mL	1.0777 mL	2.1554 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: ≥ 2.08 mg/mL (4.48 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.48 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SM1-71 (compound 5) is a potent TAK1 inhibitor, with a K_i of 160 nM, it also can covalently inhibit MKNK2, MAP2K1/2/3/4/6/7, GAK, AAK1, BMP2K, MAP3K7, MAPKAPK5, GSK3A/B, MAPK1/3, SRC, YES1, FGFR1, ZAK (MLTK), MAP3K1, LIMK1 and RSK2. SM1-71 can inhibit proliferation of multiple cancer cell lines[1][2][3].

IC_{50} & Target		
	LIMK1	RSK2

In Vitro

SM1-71 (0.001-100 μM; 72 h) potently inhibits the proliferation of H23 and Calu-6 non-small cell lung cancer cell lines with a concentration-dependent manner[1].

SM1-71 (72 h) induces potent cytotoxicity with nanomolar values for GR_{50} and negative GR_{max} values in eight of 11 cancer cell lines[2].

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

Cell Viability Assay[1]

Cell Line:	H23-KRAS^{G12C} and Calu-6-KRAS^{Q61K} cells
Concentration:	0.001, 0.01, 0.1, 1, 10, 100 μM
Incubation Time:	72 hours
Result:	Inhibited proliferation of H23-KRAS^{G12C} and Calu-6-KRAS^{Q61K} cells with IC_{50}s of 0.4 and 0.3 μM, respectively.

REFERENCES

[1]. Rao S, et, al. Leveraging Compound Promiscuity to Identify Targetable Cysteines within the Kinome. Cell Chem Biol. 2019 Jun 20; 26(6): 818-829.e9.

[2]. Rao S, et, al. A multitargeted probe-based strategy to identify signaling vulnerabilities in cancers. J Biol Chem. 2019 May 24;294(21):8664-8673.

[3]. Tan L, et, al. Structure-guided development of covalent TAK1 inhibitors. Bioorg Med Chem. 2017 Feb 1; 25(3): 838-846.

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