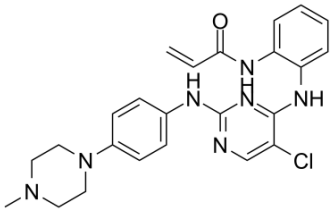
SM1-71

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:	Please store the product under the recommended conditions in the Certificate of Analysis.



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	IC50: 0.8 nM (GAK), 0.8 nM (YES1), 2 nM (SRC), 4.4 nM (AAK1), 5.4 nM (LIMK1), 7.1 nM (BMP2K), 9.3 nM (MAP2K2), 10.4 nM (MAP2K1), 28.7 nM (MAP3K1), 48.3 nM (MAPK1), 107 nM (MAPK3)[1]
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.

Caution: Product has not been fully validated for medical applications. For research use only.

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