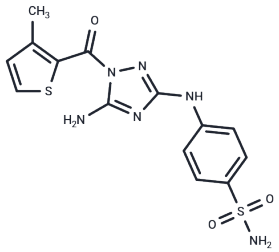
Data Sheet (Cat.No.T40546)

TargetMol

3-Methylthienyl-carbonyl-JNJ-7706621

Chemical Properties



CAS No. : 443798-09-2

Formula: C14H14N6O3S2

Molecular Weight: 378.43

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	3-Methylthienyl-carbonyl-JNJ-7706621 is a highly potent and selective inhibitor of cyclin-dependent kinase (CDK), showing IC50 values of 6.4 nM for CDK1/cyclin B and 2 nM for CDK2/cyclin A. It also exhibits potent inhibition of GSK-3 (IC50 = 0.041 μM) and moderate inhibition of CDK4, VEGF-R2, and FGF-R2 (IC50 = 0.11 μM, 0.13 μM, and 0.22 μM, respectively), making it significant for cancer research.
Targets(IC50)	FGFR,Others,CDK,GSK-3,VEGFR
In vitro	3-Methylthienyl-carbonyl-JNJ-7706621 demonstrates significant inhibitory activity against GSK-3 with an IC50 value of 0.041 μM and displays moderate inhibitory effects on CDK4, VEGF-R2, and FGF-R2 with IC50 values of 0.11 μM, 0.13 μM, and 0.22 μM, respectively[1]. Additionally, this compound effectively hinders the proliferation of various cancer cell lines, including HeLa, HCT-116, A375, SK-OV-3, MDA-MB-231, and PC-3, showcasing IC50 values of 0.28 μM, 0.25 μM, 0.45 μM, 0.75 μM, 0.59 μM, and 0.12 μM, respectively[1].
In vivo	Administering 3-Methylthienyl-carbonyl-JNJ-7706621 at dosages of 75-125 mg/kg intraperitoneally (i.p.) once daily for 32 days significantly reduced A375 human melanoma tumor growth and increased survival in male athymic nude mice. The compound demonstrated oral bioavailability in nude mice (2%), rats (8%), and dogs (63.3%), with terminal elimination half-lives of 1.70 hours in nude mice, 2.20 hours in rats, and 2.36 hours in dogs. Additionally, after oral administration at doses of 30 mg/kg for mice and rats, and 10 mg/kg for dogs, peak concentration (Cmax) values were observed at 0.21 μM in nude mice, 2.5 μM in rats, and 4.58 μM in dogs. Following intravenous administration at 3 mg/kg for mice and rats, and 1 mg/kg for dogs, the compound showed terminal elimination half-lives of 0.51 hours in nude mice, 0.64 hours in rats, and 3.89 hours in dogs. Cmax values were 6.4 μM in nude mice, 23.2 μM in rats, and 2.19 μM in dogs, while the area under the curve (AUC) was 3.2 μM·h for nude mice, 11.4 μM·h for rats, and 2.45 μM·h for dogs. The result was a notable reduction in tumor growth and an extension of survival by approximately 3 weeks compared to the control group.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6425 mL	13.2125 mL	26.425 mL
5 mM	0.5285 mL	2.6425 mL	5.285 mL
10 mM	0.2642 mL	1.3212 mL	2.6425 mL
50 mM	0.0528 mL	0.2642 mL	0.5285 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Lin R, et, al. 1-Acyl-1H-[1,2,4]triazole-3,5-diamine analogues as novel and potent anticancer cyclin-dependent kinase inhibitors: synthesis and evaluation of biological activities. J Med Chem. 2005 Jun 30;48(13):4208-11.