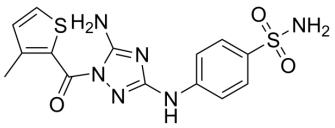
3-Methylthienyl-carbonyl-JNJ-7706621

Cat. No.:	HY-141685
CAS No.:	443798-09-2
Molecular Formula:	$C_{14}H_{14}N_6O_3S_2$
Molecular Weight:	378.43
Target:	CDK; GSK-3; VEGFR; FGFR
Pathway:	Cell Cycle/DNA Damage; PI3K/Akt/mTOR; Stem Cell/Wnt; Protein Tyrosine Kinase/RTK
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

3-Methylthienyl-carbonyl-JNJ-7706621 is a potent and selective inhibitor of cyclin-dependent kinase (CDK), with IC_{50}s of 6.4 nM and 2 nM for CDK1/cyclin B and CDK2/cyclin A, respectively. 3-Methylthienyl-carbonyl-JNJ-7706621 also shows potent inhibition of GSK-3 (IC_{50}=0.041 μM) and modest potency against CDK4, VEGF-R2, and FGF-R2 (IC_{50}=0.11, 0.13, 0.22 μM, respectively). 3-Methylthienyl-carbonyl-JNJ-7706621 can be used for the research of cancer[1].

IC_{50} & Target

CDK2/cyclinA 2 nM (IC_{50})	CDK1/cyclinB 6.4 nM (IC_{50})	GSK3 41 nM (IC_{50})	CDK4 0.11 μM (IC_{50})
VEGFR2 0.13 μM (IC_{50})	FGFR2 0.22 μM (IC_{50})		

In Vitro

3-Methylthienyl-carbonyl-JNJ-7706621 shows potent potency against GSK-3 (IC_{50}=0.041 μM) and modest potency against CDK4, VEGF-R2, and FGF-R2 (IC_{50}=0.11, 0.13, 0.22 μM, respectively)[1].

3-Methylthienyl-carbonyl-JNJ-7706621 inhibits cell proliferation, with IC_{50}s of 0.28 μM, 0.25 μM, 0.45 μM, 0.75 μM, 0.59 μM and 0.12 μM for HeLa, HCT-116, A375, SK-OV-3, MDA-MB-231 and PC-3 cells, respectively[1].

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

In Vivo

3-Methylthienyl-carbonyl-JNJ-7706621 (75-125 mg/kg; i.p. once daily for 32 days) inhibits the A375 human melanoma tumor growth and prolongs the survival in nude mice[1].

3-Methylthienyl-carbonyl-JNJ-7706621 exhibits oral bioavailability (nude mouse 2%, rat 8%, dog 63.3%), terminal elimination half-lives (nude mouse 1.70, rat 2.20 and, dog 2.36 h) and C_{max} (nude mouse 0.21, rat 2.5, dog 4.58 μM) following oral administration (nude mouse 30, rat 30 , dog 10 mg/kg)[1].

3-Methylthienyl-carbonyl-JNJ-7706621 exhibits terminal elimination half-lives (nude mouse 0.51, rat 0.64 and, dog 3.89 h), C_{max} (nude mouse 6.4, rat 23.2, dog 2.19 μM) and AUC (nude mouse 3.2, rat 11.4, dog 2.45 μM•h) following intravenous administration (nude mouse 3, rat 3 and, dog 1 mg/kg)[1].

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

Animal Model:	Male athymic mice were implanted with A375 human melanoma cells[1]
Dosage:	75, 100, 125 mg/kg
Administration:	I.p. once daily for 32 days

Result:	Reduced the tumor growth. Survival was increased by about 3 weeks compared with vector alone.

REFERENCES

[1]. 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.

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