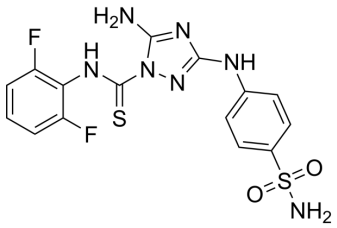
K00546

Cat. No.:	HY-103647
CAS No.:	443798-47-8
Molecular Formula:	$C_{15}H_{13}F_2N_7O_2S_2$
Molecular Weight:	425.44
Target:	CDK; GSK-3; VEGFR
Pathway:	Cell Cycle/DNA Damage; PI3K/Akt/mTOR; Stem Cell/Wnt; Protein Tyrosine Kinase/RTK



Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year

SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (235.05 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3505 mL	11.7525 mL	23.5051 mL
	5 mM	0.4701 mL	2.3505 mL	4.7010 mL
	10 mM	0.2351 mL	1.1753 mL	2.3505 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

K00546 is a potent CDK1 and CDK2 inhibitor with IC_{50}s of 0.6 nM and 0.5 nM for CDK1/cyclin B and CDK2/cyclin A, respectively. K00546 is also a potent CDC2-like kinase 1 (CLK1) and CLK3 inhibitor with IC_{50}s of 8.9 nM and 29.2 nM, respectively[1][2][3].

IC_{50} & Target

Cdk1/cyclin B 0.6 nM (IC_{50})	cdk2/cyclin A 0.5 nM (IC_{50})	CLK1 8.9 nM (IC_{50})	CLK3 29.2 nM (IC_{50})
VEGF-R2 32 nM (IC_{50})	GSK-3 140 nM (IC_{50})		

In Vitro

K00546 binds to the SLK ATP-binding site forming three hydrogen bonds with the kinase hinge residues E109 and C111. The sulphamoyl moiety of K00546 also interacts with the main chain of L40[1].

K00546 (compound 3n) also inhibits PKA, casein kinase-1, MAP kinase (ERK-2), calmodulin kinase, VEGF-R2, GSK-3 and PDGF-Rβ with IC_{50} values of 5.2 μM, 2.8 μM, 1.0 μM, 8.9 μM, 0.032 μM, 0.14 μM and 1.6 μM, respectively[2].

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

REFERENCES

[1]. Ashley C W Pike, et al. Activation segment dimerization: a mechanism for kinase autophosphorylation of non-consensus sites. EMBO J. 2008 Feb 20;27(4):704-14.

[2]. Oleg Fedorov, et al. Specific CLK inhibitors from a novel chemotype for regulation of alternative splicing. Chem Biol. 2011 Jan 28;18(1):67-76.

[3]. Ronghui Lin, 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.

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