CDK12-IN-2

Cat. No.: HY-112626

CAS No.: 2244987-03-7

Molecular Formula: $C_{32}H_{32}N_6O_2$

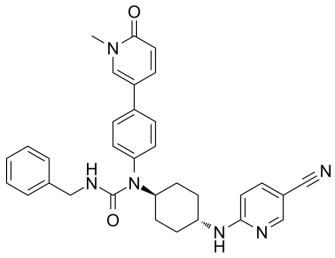
Molecular Weight: 532.64

Target: CDK

Pathway: 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 : 50 mg/mL (93.87 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8774 mL	9.3872 mL	18.7744 mL
	5 mM	0.3755 mL	1.8774 mL	3.7549 mL
	10 mM	0.1877 mL	0.9387 mL	1.8774 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: 2.5 mg/mL (4.69 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (4.69 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.69 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CDK12-IN-2 is a potent, selective and nanomolar CDK12 inhibitor (IC_{50}=52 nM) with good physicochemical properties. CDK12-IN-2 is also a strong CDK13 inhibitor due to CDK13 is the closest homologue of CDK12. CDK12-IN-2 shows excellent kinase selectivity for CDK12 over CDK2, 9, 8, and 7. CDK12-IN-2 inhibits the phosphorylation of Ser2 in the C-terminal domain of RNA polymerase II. CDK12-IN-2 can be used an excellent chemical probe for functional studies of CDK12[1].

IC_{50} & Target				
	CDK12	CDK2	CDK7	CDK7
	52 nM (IC_{50})	>100 μM (IC_{50})	>10 μM (IC_{50})	>10 μM (IC_{50})

	CDK9 16 μM (IC_{50})
In Vitro	CDK12-IN-2 inhibits the phosphorylation of the CTD Ser2 in SK-BR-3 cells at low submicromolar concentrations, it inhibits C-terminal domain ser2 phosphorylation with an IC_{50} of 185 nM. And CDK12-IN-2 exhibits a growth inhibition with an IC_{50} of 0.8 μM in SK-BR-3 cells[1]. CDK12-IN-2 exhibits time dependency for CDK12 inhibition, the IC_{50} value for CDK12-IN-2 are 0.0078 μM, 0.042 μM, 0.057 μM,and 0.059 μM, for 0h, 1h, 2h and 5h respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Masahiro Ito, et al. Discovery of 3-Benzyl-1-(trans-4-((5-cyanopyridin-2-yl)amino)cyclohexyl)-1-arylurea Derivatives as Novel and Selective Cyclin-Dependent Kinase 12 (CDK12) Inhibitors. J Med Chem. 2018 Sep 13;61(17):7710-7728.

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