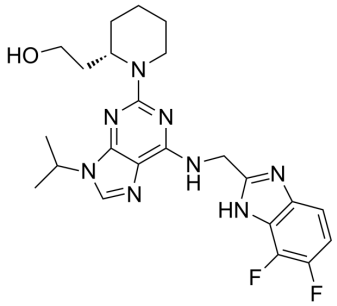
CDK12-IN-3

Cat. No.:	HY-112261
CAS No.:	2220184-50-7
Molecular Formula:	$C_{23}H_{28}F_2N_8O$
Molecular Weight:	470.52
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
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 : 250 mg/mL (531.33 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1253 mL	10.6265 mL	21.2531 mL
	5 mM	0.4251 mL	2.1253 mL	4.2506 mL
	10 mM	0.2125 mL	1.0627 mL	2.1253 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: ≥ 2.33 mg/mL (4.95 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.33 mg/mL (4.95 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CDK12-IN-3 is a potent and selective CDK12 inhibitor with an IC_{50} of 491 nM in enzymatic assay.

IC_{50} & Target

CDK12
491 nM (IC_{50})

In Vitro

CDK12-IN-3 is a highly selective CDK12 inhibitor. CDK12-IN-3 (0.1 μM) shows potent inhibition of phosphorylation of Ser2 on the CTD repeat domain of RNA Pol II as well as growth inhibition of OV90 cells and acute cytotoxicity to THP1 cells.[1].

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

REFERENCES

[1]. Johannes JW, et al. Structure-Based Design of Selective Noncovalent CDK12 Inhibitors. ChemMedChem. 2018 Feb 6;13(3):231-235.

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