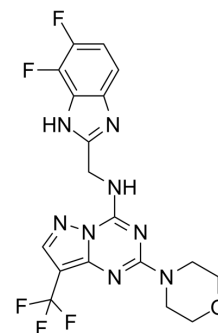


CDK12-IN-5

Cat. No.:	HY-139328		
CAS No.:	2651200-35-8		
Molecular Formula:	C ₁₈ H ₁₅ F ₅ N ₈ O		
Molecular Weight:	454.36		
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 : 125 mg/mL (275.11 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	2.2009 mL	11.0045 mL	22.0090 mL
		5 mM	0.4402 mL	2.2009 mL	4.4018 mL
10 mM		0.2201 mL	1.1004 mL	2.2009 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: 2.08 mg/mL (4.58 mM); Suspended solution; Need ultrasonic 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.58 mM); Clear solution				

BIOLOGICAL ACTIVITY

Description	CDK12-IN-5, a pyrazolotriazine, is a potent CDK12 inhibitor with an IC ₅₀ of 23.9 nM at high ATP (2 mM). CDK12-IN-5 has no effect on CDK2/Cyclin E (IC ₅₀ =173 μM) and CDK9/Cyclin T1 (IC ₅₀ =127 μM) at high ATP (2 mM) (WO2021116178A1) ^[1] .		
IC₅₀ & Target	CDK12 23.9 nM (IC ₅₀)	CDK2/cyclinE 173 μM (IC ₅₀)	CDK9/cyclinT1 127 μM (IC ₅₀)
In Vitro	CDK12-IN-5 (Example 426) inhibits BRCA1 mRNA expression in MDA-MB-231 cells (IC ₅₀ =3.23 nM) and has no effect on CAL-120 cells ^[1] . CDK12-IN-5 has antiproliferative activity in MDA-MB-231 cells (IC ₅₀ =4.19 nM) and CAL-120 cells (IC ₅₀ =3.57 nM) ^[1] . CDK12-IN-5 has a inhibition IC ₅₀ CDK12 high ATP to Degradation DC ₅₀ CDK12 ratio of 32 ^[1] .		

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

REFERENCES

[1]. Kai Thede, et al. Pyrazolotriazines. WO2021116178A1.

Caution: Product has not been fully validated for medical applications. For research use only.

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