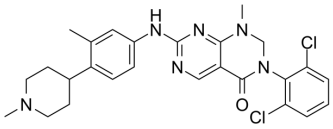
WEE1-IN-5

Cat. No.:	HY-147054
CAS No.:	2243882-74-6
Molecular Formula:	$C_{26}H_{28}Cl_2N_6O$
Molecular Weight:	511.45
Target:	Wee1; 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 : 20 mg/mL (39.10 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9552 mL	9.7761 mL	19.5523 mL
	5 mM	0.3910 mL	1.9552 mL	3.9105 mL
	10 mM	0.1955 mL	0.9776 mL	1.9552 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: ≥ 1 mg/mL (1.96 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1 mg/mL (1.96 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1 mg/mL (1.96 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

WEE1-IN-5 is a potent WEE1 inhibitor with an IC_{50} value of 0.8 nM. WEE1-IN-5 inhibits phospho-CDC2. WEE1-IN-5 abrogates the G2 check point, increasing sensitivity to DNA damaging agents in cancer cells. WEE1-IN-5 can be used for researching anticancer[1].

IC_{50} & Target

IC_{50}: 0.8 nM (WEE1), 188 nM (CDC2)[1]

In Vitro

WEE1-IN-5 exhibits an EC_{50} of 188 nM in pCDC2 and an IC_{50} shift for CYP3A4/5[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	WEE1-IN-5 (5mg/kg for PO; 1 mg/kg for IV; single dosage) exhibits a CL of 14 mL/min/kg, an AUC_{int} 1324 h·ng/mL and bioavailability of 35% in SD rats[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. H. Gelderblom, et al. 601TiP First-in-human phase I study of a novel oral Wee1 inhibitor (Debio 0123) in combination with carboplatin in patients with advanced solid tumours. Ann Oncol. 2020 Sep; 31: S501-S502.

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