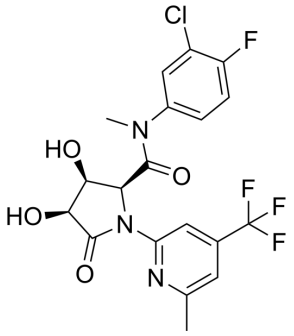
ART812

Cat. No.:	HY-139289
CAS No.:	2607138-82-7
Molecular Formula:	$C_{19}H_{16}ClF_4N_3O_4$
Molecular Weight:	461.79
Target:	DNA/RNA Synthesis
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 : 100 mg/mL (216.55 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1655 mL	10.8274 mL	21.6549 mL
	5 mM	0.4331 mL	2.1655 mL	4.3310 mL
	10 mM	0.2165 mL	1.0827 mL	2.1655 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 (5.41 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.41 mM); Suspended solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.41 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ART812 is an orally active DNA polymerase Polθ inhibitor with an IC_{50} value of 7.6 nM. ART812 has an IC_{50} value of 240 nM for cell based microhomology-mediated end joining (MMEJ)[1][2].

IC_{50} & Target

Polθ
7.6 nM (IC_{50})

In Vitro

ART812 (0-40 μM) elicits Polθ inhibitor sensitivity in MDA-MB-436 SHLD2 knockout cells[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ART812 (100 mg/kg; p.o. daily for 76 days) shows significant tumour inhibition in rats bearing established MDA-MB-436 BRCA1/SHLD2 defective tumours (volume 250-350 mm^3)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Zatreanu D, et al. Polθ inhibitors elicit BRCA-gene synthetic lethality and target PARP inhibitor resistance. Nat Commun. 2021 Jun 17;12(1):3636.

[2]. Peter BLENCOWE, et al. Preparation of heterocyclic compounds for use in the treatment of cancer. WO2021028643 A1.

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