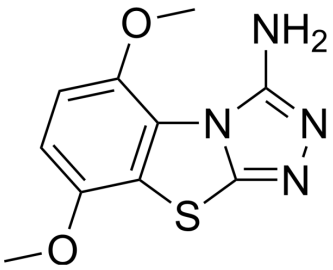
OUL232

Cat. No.:	HY-148566
CAS No.:	943119-42-4
Molecular Formula:	$C_{10}H_{10}N_4O_2S$
Molecular Weight:	250.28
Target:	PARP
Pathway:	Cell Cycle/DNA Damage; Epigenetics
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 (199.78 mM; ultrasonic and warming and adjust pH to 2 with 1M HCl and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.9955 mL	19.9776 mL	39.9552 mL
	5 mM	0.7991 mL	3.9955 mL	7.9911 mL
	10 mM	0.3996 mL	1.9978 mL	3.9955 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: 5 mg/mL (19.98 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 5 mg/mL (19.98 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

OUL232 is a potent inhibitor of mono-ARTs PARP7, PARP10, PARP11, PARP12, PARP14, and PARP15. OUL232 is the most potent PARP10 inhibitor described to date (IC_{50}=7.8 nM), as well as the first PARP12 inhibitor ever reported[1].

IC_{50} & Target

PARP7 83 nM (IC_{50})	PARP10 7.8 nM (IC_{50})	PARP14 300 nM (IC_{50})	PARP15 56 nM (IC_{50})
PARP1 15 μM (IC_{50})	PARP2 10 μM (IC_{50})	PARP3 50 μM (IC_{50})	PARP4 11 μM (IC_{50})
TNKS1	TNKS2	PARP11	PARP12

	5.4 μM (IC_{50})	10 μM (IC_{50})	240 nM (IC_{50})	160 nM (IC_{50})
	PARP16 3.4 μM (IC_{50})			

In Vitro

OUL232 (compound 27) (1 μM; 10-12 d) saves cells overexpressing PARP10 from ADP ribosylation-dependent cell death[1].

Pharmacokinetic Analysis[1]

water solubility μg/mL	GI P_{app}×10^{-6} cm/s (RM %)	BBB P_{app}×10^{-6} cm/s (RM %)	metabolic stablity %	stab in human plasma	stab. in MeOH	stab in PBS pH 7.4
12.60	0.144	0.143	99.11	>24	>24	>24

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

REFERENCES

[1]. Murthy S, et al. [1,2,4]Triazolo[3,4-b]benzothiazole Scaffold as Versatile Nicotinamide Mimic Allowing Nanomolar Inhibition of Different PARP Enzymes. J Med Chem. 2023 Jan 4.

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