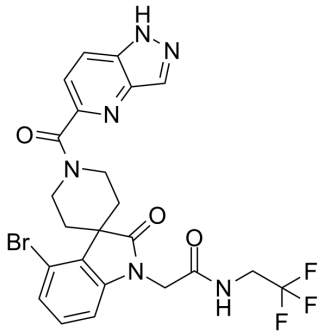
DDR1-IN-4

Cat. No.:	HY-114173
CAS No.:	2125676-13-1
Molecular Formula:	$C_{23}H_{20}BrF_3N_6O_3$
Molecular Weight:	565.34
Target:	Discoidin Domain Receptor
Pathway:	Protein Tyrosine Kinase/RTK
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 : 250 mg/mL (442.21 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7688 mL	8.8442 mL	17.6885 mL
	5 mM	0.3538 mL	1.7688 mL	3.5377 mL
	10 mM	0.1769 mL	0.8844 mL	1.7688 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.68 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.68 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DDR1-IN-4 (Compound 2.45) is a selective and potent Discoidin Domain Receptor 1 (DDR1) autophosphorylation inhibitor, with IC_{50} values of 29 nM and 1.9 μM for DDR1 and DDR2, respectively[1].

IC_{50} & Target

DDR1	DDR2
29 nM (IC_{50})	1900 nM (IC_{50})

In Vitro

DDR1-IN-4 (Compound 2.45) shows a clear dose-dependent inhibition of DDR1 phosphorylation in HT1080 cells overexpressing DDR1, with greater than 70% inhibition of phosphorylation at a concentration of 1 μM, and retaining selectivity over inhibition of DDR2[1].

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

In Vivo

DDR1-IN-4 (Compound 2.45, ip, 90 mg/kg) preserves renal function and reduces tissue damage in Col4a3$^{-/-}$ mice (the preclinical mouse model of Alport syndrome) when employing a therapeutic dosing regime, indicating the real therapeutic value of selectively inhibiting DDR1 phosphorylation in vivo[1].

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

Animal Model:	Col4a3$^{-/-}$ mice, a mouse model phenocopying Alport syndrome[1].
Dosage:	90 mg/kg.
Administration:	Injected intraperitoneally daily.
Result:	Resulted in a significant reduction of fibrosis evaluated by Picro Sirius Red, smooth muscle actin staining, and collagen I accumulation. Significantly reduces the levels of pDDR1 in Col4a3 knockout mice compared to controls.

REFERENCES

[1]. Hans Richter, et al. DNA-Encoded Library-Derived DDR1 Inhibitor Prevents Fibrosis and Renal Function Loss in a Genetic Mouse Model of Alport Syndrome. ACS Chem Biol. 2019 Jan 18;14(1):37-49.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA