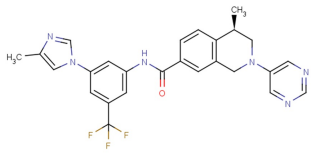
Data Sheet (Cat.No.T10984)

TargetMol
A DRUG SCREENING EXPERT

DDR-TRK-1

Chemical Properties



CAS No.:	1934246-19-1
Formula:	C26H23F3N6O
Molecular Weight:	492.5
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	DDR-TRK-1 is a selective discoid domain receptor 1 (DDR1) inhibitor with IC50 value of 9.4 nM. DDR-TRK-1 also inhibits the TRK family.
Targets(IC_{50})	DDR1: 9.4 nM
In vitro	DDR-TRK-1 is a promising candidate with an IC50 value of 9.4 nM relative to DDR1. DDR-TRK-1 also exhibited reasonable pharmacokinetic (PK) properties. At an oral dose of 20 mg/kg in rats, the oral bioavailability was 66.8%, and the T1/2 value was 1.25 h. However, the area under the concentration-time curve (AUC) value of DDR-TRK-1 in mice was significantly higher than that in rats, indicating that its absorption performance in mice was good. By determining the binding affinity of DDR1-IN-3 and DDR1 protein, the inhibitory effect of DDR1 on DDR1-IN-3 can be further verified. The results show that DDR-TRK-1 is closely bound to DDR1, and the binding constant (Kd) value is 4.7 nM.
In vivo	DDR-TRK-1 can prevent blm-induced pathological changes in a dose-dependent manner. These results agree with the expression levels of fibrosis markers in the lung tissue, including lysates, including fibronectin and α-smooth muscle actin (SMA). Further analysis also showed that the use of DDR-TRK-1 resulted in a dose-dependent inhibition of hydroxyproline content, a unique amino acid found in collagen. The above data indicate that DDR-TRK-1 has good therapeutic potential for blm-induced pulmonary fibrosis.

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.03 mL	10.152 mL	20.305 mL
5 mM	0.406 mL	2.03 mL	4.061 mL
10 mM	0.203 mL	1.015 mL	2.03 mL
50 mM	0.041 mL	0.203 mL	0.406 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Zhen Wang, et al. Structure-Based Design of Tetrahydroisoquinoline-7-carboxamides as Selective Discoidin Domain Receptor 1 (DDR1) Inhibitors. J Med Chem. 2016 Jun 23; 59(12): 5911–5916.

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