SK1-IN-1

Cat. No.: HY-101805

CAS No.: 1218816-71-7

Molecular Formula: $C_{22}H_{30}N_4O_3$

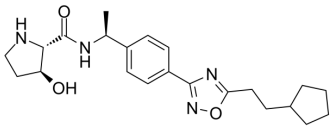
Molecular Weight: 398.5

Target: SphK

Pathway: Immunology/Inflammation

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (250.94 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.5094 mL	12.5471 mL	25.0941 mL
5 mM	0.5019 mL	2.5094 mL	5.0188 mL
10 mM	0.2509 mL	1.2547 mL	2.5094 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 (6.27 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.27 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.27 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SK1-IN-1 is a potent sphingosine kinase 1 (SPHK1) inhibitor with an IC_{50} of 58 nM.

IC_{50} & Target

IC50: 58 nM (SPHK1)[1]

In Vivo

SK1-IN-1 demonstrates significant improvement in the intrinsic clearance, particularly against human liver microsomes. SK1-IN-1 is selected for rat PK studies and demonstrates modest in oral bioavailability with acceptable half-lives in blood

circulation[1].

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

CUSTOMER VALIDATION

- Cell Res. 2022 Feb 1.

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REFERENCES

[1]. Xiang Y, et al. Discovery of novel sphingosine kinase-1 inhibitors. Part 2. Bioorg Med Chem Lett. 2010 Aug 1;20(15):4550-4.

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