Proteins

TP0472993

Cat. No.: HY-151810 CAS No.: 2126874-77-7 Molecular Formula: $C_{16}H_{20}N_4O_2$ Molecular Weight: 300.36

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light

* In solvent: -80°C, 6 months; -20°C, 1 month (protect from light)

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 25 mg/mL (83.23 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.3293 mL	16.6467 mL	33.2934 mL
	5 mM	0.6659 mL	3.3293 mL	6.6587 mL
	10 mM	0.3329 mL	1.6647 mL	3.3293 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 (8.32 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (8.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	CYP4A11/CYP4F2-IN-2 is a potent and orally active dual inhibitor of cytochrome P450 (CYP) 4A11 and CYP4F2, with IC ₅₀ s of 140 nM and 40 nM, respectively. CYP4A11/CYP4F2-IN-2 has potential for the research of renal diseases ^[1] .		
IC ₅₀ & Target	CYP4A11 140 nM (IC ₅₀)	CYP4F2 40 nM (IC ₅₀)	
In Vitro	CYP4A11/CYP4F2-IN-2 (compound 11c) inhibits 20-Hydroxyeicosatetraenoic acid (20-HETE) production from arachidonic acid in human renal microsomes, with an IC $_{50}$ of 29 nM $^{[1]}$. MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
In Vivo	CYP4A11/CYP4F2-IN-2 (compound 11c) (0.03-1 mg/kg; a single p.o.) inhibits renal 20-HETE production of rats in a dose-		

dependent manner[1].

CYP4A11/CYP4F2-IN-2 (0.5 mg/kg; i.v.) exhibits low CL (1430 mL/h/kg), moderate V_{dss} (763 mL/kg), and short $T_{1/2}$ (0.424 h) in mice^[1].

CYP4A11/CYP4F2-IN-2 (1 mg/kg; i.v.) exhibits low CL (226 mL/h/kg), moderate $V_{dss}(839 \text{ mL/kg})$, and $T_{1/2}$ (3.01 h) in SD rats^[1]. CYP4A11/CYP4F2-IN-2 (1 mg/kg; p.o.) exhibits C_{max} (623 ng/mL), $T_{1/2}$ (3.03 h), and high bioavailability (97.7%) in SD rats^[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Kawamura M, et, al. Discovery of Novel Pyrazolylpyridine Derivatives for 20-Hydroxyeicosatetraenoic Acid Synthase Inhibitors with Selective CYP4A11/4F2 Inhibition. J Med Chem. 2022 Nov 10;65(21):14599-14613.

Caution: Product has not been fully validated for medical applications. For research use only.

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Page 2 of 2 www.MedChemExpress.com