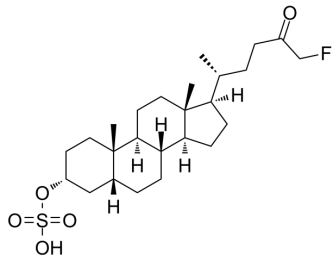
AAA-10

Cat. No.:	HY-145147
CAS No.:	2758171-70-7
Molecular Formula:	$C_{25}H_{41}FO_5S$
Molecular Weight:	472.65
Target:	Bacterial
Pathway:	Anti-infection
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 (105.79 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1157 mL	10.5787 mL	21.1573 mL
	5 mM	0.4231 mL	2.1157 mL	4.2315 mL
	10 mM	0.2116 mL	1.0579 mL	2.1157 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 (5.29 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.29 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.29 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

AAA-10 is an orally active gut bacterial bile salt hydrolases (BSH) inhibitor, with IC_{50}s of 10 nM, 80 nM against B. theta rBSH and B. longum rBSH respectively[1].

IC_{50} & Target

IC50: 10 nM (B. theta rBSH), 80 nM (B. longum rBSH)[1]

In Vitro

AAA-10 (100 μM; 24 h) inhibits BSH activity in bacterial cultures, with IC_{50}s of 74 nM, 901 nM for Gram-negative and Gram-positive bacteria, respectively[1].

	AAA-10 (20 μM; 2 h) significantly inhibits deconjugation of glycochenodeoxycholic acid-d4 or taurocholic acid-d4 substrates of human feces[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	AAA-10 (30 mg/kg; orally gavage daily for 5 days) decreases the abundances of deoxycholic acid (DCA) and lithocholic acid (LCA) in mice feces starting in day 2-5[1]. AAA-10 (30 mg/kg) displays high colonic exposure and low gut permeability[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	10-11 weeks old male C57Bl/6J mice[1]
Dosage:	30 mg/kg
Administration:	Orally gavaged once daily for 5 days
Result:	Decreased the abundances of DCA and LCA in mice feces starting in day 2-5. Displayed high colonic exposure and low gut permeability.

REFERENCES

[1]. Adhikari AA, et al. A Gut-Restricted Lithocholic Acid Analog as an Inhibitor of Gut Bacterial Bile Salt Hydrolases. ACS Chem Biol. 2021;16(8):1401-1412.

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