AAA-10 formic

Cat. No.: HY-145147A

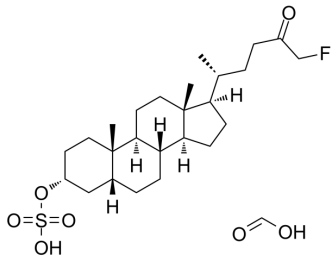
Molecular Formula: $C_{26}H_{43}FO_7S$

Molecular Weight: 518.68

Target: Bacterial

Pathway: Anti-infection

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



SOLVENT & SOLUBILITY

In Vitro

DMSO : 16.67 mg/mL (32.14 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9280 mL	9.6399 mL	19.2797 mL
	5 mM	0.3856 mL	1.9280 mL	3.8559 mL
	10 mM	0.1928 mL	0.9640 mL	1.9280 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: ≥ 1.67 mg/mL (3.22 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.67 mg/mL (3.22 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.67 mg/mL (3.22 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

AAA-10 formic 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) formic 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) formic 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) formic 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) formic 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.

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

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