BSH-IN-1

Cat. No.: HY-135659

CAS No.: 2553217-91-5

Molecular Formula: $C_{25}H_{41}FO_3$

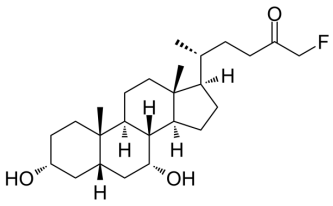
Molecular Weight: 408.59

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 : 25 mg/mL (61.19 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4474 mL	12.2372 mL	24.4744 mL
	5 mM	0.4895 mL	2.4474 mL	4.8949 mL
	10 mM	0.2447 mL	1.2237 mL	2.4474 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 (6.12 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.12 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.12 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BSH-IN-1 is a potent and covalent inhibitor of gut bacterial recombinant bile salt hydrolases (BSHs) with IC_{50}s of 108 nM and 427 nM for B. longum BSH (Gram positive) and B. theta BSH (Gram negative), respectively[1].

In Vitro

BSH-IN-1 (Compound 7) also inhibits BSH activity in growing cultures of Gram-negative (B. theta VPI-5482, Bacteroides fragilis ATCC 25285, and Bacteroides vulgatus ATCC 8482) and Gram-positive (Lactobacillus plantarum WCFS1, C. perfringens ATCC 13124, and Bifidobacterium adolescentis L2-32) bacteria. BSH-IN-1 (Compound 7) also is a potent BSH inhibitor in growing bacterial cultures with IC_{50}s of 237 nM and 1070 nM for B. adolescentis (Gram positive) and B. theta

	(Gram negative), respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BSH-IN-1 (Compound 7; 10 mg/kg; a single dose; gavage) inhibits BSH activity in C57BL/6 mice and can be gut-restricted[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	C57BL/6 mice[1]
Dosage:	10 mg/kg
Administration:	Single gavage
Result:	Inhibited gut bacterial BSH activity and modulated the bile acid pool in vivo while not significantly affected the gut bacterial community.

REFERENCES

[1]. Adhikari AA, et al. Development of a covalent inhibitor of gut bacterial bile salt hydrolases.Nat Chem Biol. 2020 Mar;16(3):318-326.

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