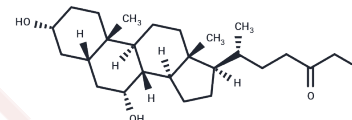


BSH-IN-1

Chemical Properties

CAS No. :	2553217-91-5
Formula:	C ₂₅ H ₄₁ F _O ₃
Molecular Weight:	408.59
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



Biological Description

Description	BSH-IN-1 is a potent, covalent inhibitor of gut bacterial recombinant bile salt hydrolases (BSHs; IC ₅₀ s: 108 nM for <i>B. longum</i> BSH and 427 nM for <i>B. theta</i> BSH).
Targets(IC ₅₀)	Antibacterial, Potassium Channel
In vitro	BSH-IN-1 also inhibits BSH activity in growing cultures of Gram-negative (<i>Bacteroides fragilis</i> ATCC 25285, <i>B. theta</i> VPI-5482, and <i>Bacteroides vulgatus</i> ATCC 8482) and Gram-positive (<i>C. perfringens</i> ATCC 13124, <i>Lactobacillus plantarum</i> WCFS1, and <i>Bifidobacterium adolescentis</i> L2-32) bacteria. BSH-IN-1 also is a potent BSH inhibitor in growing bacterial cultures with IC ₅₀ s of 237 nM and 1070 nM for <i>B. adolescentis</i> and <i>B. theta</i> , respectively.
In vivo	In C57BL/6 mice, BSH-IN-1 (10mg/kg; a single dose; gavage) inhibits BSH activity and can be gut-restricted.

Solubility Information

Solubility	DMSO: 40 mg/mL (97.9 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.89 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0489 mL	0.2447 mL	0.4895 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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