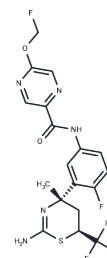


BACE1-IN-5

Chemical Properties

CAS No. :	2581114-83-0
Formula:	C ₁₈ H ₁₆ F ₅ N ₅ O ₂ S
Molecular Weight:	461.41
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	BACE1-IN-5 (Compound 15), a potent β -site amyloid precursor protein cleaving enzyme 1 (BACE1) inhibitor, demonstrates significant efficacy with an IC ₅₀ of 9.1 nM for BACE1 inhibition and an impressive IC ₅₀ of 0.82 nM against cellular amyloid- β (A β) production. Additionally, it is engineered to enhance hERG inhibition and P-gp efflux, indicating its optimized medicinal chemistry profile [1].
Targets(IC ₅₀)	Beta Amyloid,Beta-Secretase,BACE
In vivo	Treatment with BACE1-IN-5 (Compound 15), administered orally at doses ranging from 1-3 mg/kg to male ICR mice for durations of 2-6 hours, significantly and dose-dependently decreases total amyloid-beta (A β) levels. At a dose of 1 mg/kg, it reduces total A β by 76% within 4 hours, correlating with a free brain concentration of 4.1 ng/mL (8.9 nM). This compound also exhibits a K _{p,uu} value of 1.3 at the 4-hour mark and a 1 mg/kg dose. When the dosage is increased to 3 mg/kg, BACE1-IN-5 achieves a maximal A β reduction of 87%, corresponding to a free brain concentration of 9.5 ng/mL (21 nM).

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1673 mL	10.8363 mL	21.6727 mL
5 mM	0.4335 mL	2.1673 mL	4.3345 mL
10 mM	0.2167 mL	1.0836 mL	2.1673 mL
50 mM	0.0433 mL	0.2167 mL	0.4335 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

Kusakabe KI, et al. Trifluoromethyl Dihydrothiazine-Based β -Secretase (BACE1) Inhibitors with Robust Central A β Reduction and Minimal Covalent Binding Burden. ChemMedChem. 2019 Oct 27.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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