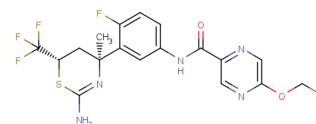


BACE1-IN-5

Chemical Properties

CAS No.:	T10453
Formula:	C ₁₈ H ₁₆ F ₅ N ₅ O ₂ S
Molecular Weight:	461.41
Appearance:	N/A
Storage:	0-4°C for short term (days to weeks), or -20°C for long term (months).



Biological Description

Description	BACE1-IN-5 is a BACE1 inhibitor (IC ₅₀ : 9.1 nM) and also inhibits cellular amyloid- β (A β ; IC ₅₀ : 0.82 nM). BACE1-IN-5 has medicinal chemistry that improves hERG inhibition and P-gp efflux.
Targets(IC ₅₀)	BACE1: 9.1 nM cellular amyloid- β : 0.82 nM
In vivo	BACE1-IN-5 (Compound 15; 1-3 mg/kg; p.o.; for 2-6 hours; male ICR mice) treatment results in a significant and dose-dependent decrease of total A β , reduces total A β by 76% (4 hours) at a free brain concentration of 4.1 ng/mL (8.9 nM) at 1 mg/kg. BACE1-IN-5 demonstrates a K(p,uu) value of 1.3 at 1 mg/kg (4 hours time point). At 3 mg/kg, a maximum A β reduction of 87% is achieved at a free brain concentration of 9.5 ng/mL (21 nM).

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.167 mL	10.836 mL	21.673 mL
5 mM	0.433 mL	2.167 mL	4.335 mL
10 mM	0.217 mL	1.084 mL	2.167 mL
50 mM	0.043 mL	0.217 mL	0.433 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 °C for 6 months; - 20 °C for 1 month. Please use it as soon as possible.

Reference

1. 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.

Inhibitors · Natural Compounds · Compound Libraries

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