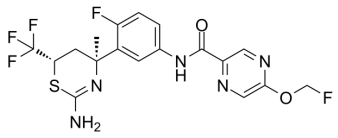
BACE1-IN-5

Cat. No.:	HY-130244
CAS No.:	2581114-83-0
Molecular Formula:	$C_{18}H_{16}F_5N_5O_2S$
Molecular Weight:	461.41
Target:	Beta-secretase
Pathway:	Neuronal Signaling
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	BACE1-IN-5 (Compound 15) is a β-site amyloid precursor protein cleaving enzyme 1 (BACE1) inhibitor with an IC_{50} of 9.1 nM, and also inhibits cellular amyloid-β (Aβ) with an IC_{50} of 0.82 nM. BACE1-IN-5 has a medicinal chemistry that improves hERG inhibition and P-gp efflux[1].
IC_{50} & Target	BACE1
In Vivo	BACE1-IN-5 (Compound 15; 1-3 mg/kg; oral administration; for 2-6 hours; male ICR mice) treatment results in a significant and dose-dependent decrease of total Aβ, reduces total Aβ by 76% (4 hours) at a free brain concentration of 4.1 ng/mL (8.9 nM) at 1 mg/kg. BACE1-IN-5 demonstrats a $K_{p,uu}$ value of 1.3 at 1 mg/kg (4 hours time point). At 3 mg/kg, a maximum Aβ reduction of 87% is achieved at a free brain concentration of 9.5 ng/mL (21 nM) [1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male ICR mice[1]
Dosage:	1 mg/kg, 3 mg/kg
Administration:	Oral administration; for 2 hours, 4 hours, and 6 hours
Result:	A significant and dose-dependent decrease of total Aβ was seen, reduced total Aβ by 76% (4 h) at a free brain concentration of 4.1 ng/mL (8.9 nM) at 1 mg/kg. Demonstrats a $K_{p,uu}$ value close to 1 ($K_{p,uu}$ of 1.3) at 1 mg/kg (4 h time point). At 3 mg/kg, a maximum Aβ reduction of 87% was achieved at a free brain concentration of 9.5 ng/mL (21 nM).

REFERENCES

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

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

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