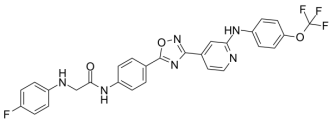
BuChE-IN-2

Cat. No.:	HY-143413
CAS No.:	2745118-93-6
Molecular Formula:	$C_{28}H_{20}F_4N_6O_3$
Molecular Weight:	564.49
Target:	Amyloid-β
Pathway:	Neuronal Signaling
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	BuChE-IN-2 is an excellent butyrylcholinesterase (BuChE) inhibitor (IC_{50}s of 1.28 μM and 0.67 μM for BuChE and NO). BuChE-IN-2 can inhibit the aggregation of Aβ, ROS formation and chelate Cu^{2+}, exhibiting proper blood-brain barrier (BBB) penetration. BuChE-IN-2 has potential to research Alzheimer's disease[1].
IC_{50} & Target	IC_{50}: 1.28 μM (BuChE), 0.67 μM (NO)[1]
In Vitro	BuChE-IN-2 (compound f9) (5-50 μM; 24 hours) shows obvious neuroprotection on H_2O_2-induced PC12 cells at 20 μM[1]. BuChE-IN-2 (100 μM; 48 hours) can inhibit Aβ aggregation[1]. BuChE-IN-2 (0.1-20 μM; 24 hours) has the obviously inhibitory effect on the secretion of inflammatory factors and IL-1β (IC_{50} =1.61 μM) and TNF-α (IC_{50}=4.15 μM) in BV2 cells[1]. BuChE-IN-2 (1-10 μM; 1 hour) can significantly reduce the expression of COX-2 and iNOS in a concentration-dependent manner[1]. BuChE-IN-2 (1-50 μM; 6 hours) has a significant inhibitory effect on ROS accumulation at 20 μM[1]. BuChE-IN-2 (10-1000 μM; 2 hours) decreases the DPPH concentration dramatically from 86.09% to 34.62% when the concentration of BuChE-IN-2 increases from 10 μM to 1000 μM[1]. BuChE-IN-2 (75 μM; 2 hours; MDCKII-MDR1 cells) exhibits proper blood-brain barrier permeability[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay

Cell Line:	PC12 cells[1]
Concentration:	5, 20, 25, 50 μM
Incubation Time:	24 hour
Result:	Showed obvious neuroprotection on H_2O_2-induced PC12 cells at 20 μM.

Western Blot Analysis

Cell Line:	BV2 cells[1]
Concentration:	1, 3, and 10 μM
Incubation Time:	1 hour

Result:	Significantly reduced the expression of COX-2 and iNOS in a concentration-dependent manner.

In Vivo

BuChE-IN-2 (40.96-100 mg/kg; i.g., single) shows LD_{50} of 75.372 mg/kg in mice[1].

BuChE-IN-2 (10 and 30 mg/kg; i.g., single) can remarkably improve the cognitive impairment in scopolamine-induced mouse models according to Morris water maze experiment[1].

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

Animal Model:	Male C57BL mice (8-week-old, 18-23 g)[1]
Dosage:	100, 80, 64, 51.2, 40.96 mg/kg
Administration:	i.g.; single
Result:	The median Lethal Dose (LD_{50}) of BuChE-IN-2 was 75.372 (62.383-101.673) mg/kg (95% confidence limit).

Animal Model:	Male C57BL mice (8-week-old, 18-23 g)[1]
Dosage:	30 mg/kg, 10 mg/kg
Administration:	i.g., single
Result:	BuChE-IN-2 could remarkably improve the cognitive impairment in scopolamine-induced mouse models according to Morris water maze experiment.

REFERENCES

[1]. Liu T, et al. Design, synthesis, and biological evaluation of novel (4-(1,2,4-oxadiazol-5-yl)phenyl)-2-aminoacetamide derivatives as multifunctional agents for the treatment of Alzheimer's disease. Eur J Med Chem. 2022;227:113973.

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