

BuChE-IN-20

Chemical Properties

CAS No. :

Formula:

Molecular Weight:

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	BuChE-IN-20 is a selective hBuChE inhibitor (IC ₅₀ = 0.13 μM) with the ability to cross the blood-brain barrier (BBB). This compound, a derivative of L-Tryptophan, exhibits neuroprotective effects by inhibiting nitric oxide (NO) production and reducing reactive oxygen species (ROS) levels. It effectively suppresses the self-aggregation of amyloid-beta (Aβ) peptides and is applicable in Alzheimer's disease research.
Targets(IC50)	Beta Amyloid, Reactive Oxygen Species, NOD-like Receptor (NLR), Cholinesterase (ChE), Interleukin, ROS
In vitro	BuChE-IN-20 (Compound 4d-13) demonstrates selectivity for BuChE over hAChE when analyzed for enzyme activity at a concentration of 5 μM for 10 minutes. At 20 μM for 48 hours, it prevents the aggregation and deposition of Aβ 1-42, offering neuroprotection by inhibiting amyloid plaque formation and reducing neurotoxicity induced by Aβ 1-42 and ROS. This compound possesses a hydroxyl radical scavenging ability 775 times greater than that of Vitamin C at 1 mM for 30 minutes. BuChE-IN-20 also reduces ROS in a concentration-dependent manner in LPS (1.5 μg/mL)-induced RAW264.7 cells with 5-10 μM for 4 hours of pretreatment and an additional 8 hours of LPS treatment. Furthermore, it effectively inhibits NO production in LPS (2 μg/mL)-induced RAW264.7 cells at concentrations of 6.25-12.5 μM, with 4 hours of pretreatment followed by 24 hours of LPS co-treatment. In mouse BV-2 cell lines, BuChE-IN-20 exhibits inhibitory and radical scavenging effects at submicromolar concentrations over 24 hours, with a safety margin close to 150-fold. When pretreated for 24 hours and co-treated for 24 hours with LPS (100 ng/ml), concentrations of 1-10 μM of BuChE-IN-20 reduce IL-1β levels in BV-2 cells. Lastly, for NMDA (20 mM)/Sodium L-Glutamate(Glu)-induced SH-SY5Y cell injury models, BuChE-IN-20 at 1-20 μM, with 6 hours of pretreatment and administration 6 hours before and for 24 hours following NMDA/L-Glutamate treatment, mitigates cytotoxic effects in a dose-dependent manner.
In vivo	BuChE-IN-20 (Compound 4d-13), when administered orally as a single dose at 10-100 mg/kg, exhibited a maximum tolerated dose of 100 mg/kg in ICR mice without causing toxicity or abnormal symptoms. At doses of 10-40 mg/kg, BuChE-IN-20 significantly improved learning and memory functions impaired by (-)-Scopolamine hydrobromide (3 mg/kg, intraperitoneal injection) in ICR mice.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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