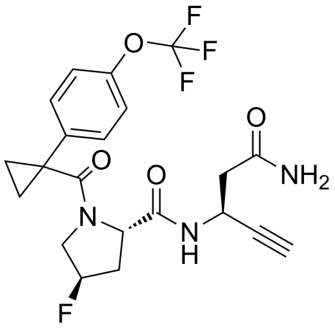
AEP-IN-3

Cat. No.:	HY-162076
CAS No.:	2978521-26-3
Molecular Formula:	$C_{21}H_{21}F_4N_3O_4$
Molecular Weight:	455.4
Target:	Others
Pathway:	Others

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (219.59 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1959 mL	10.9794 mL	21.9587 mL
5 mM	0.4392 mL	2.1959 mL	4.3917 mL
10 mM	0.2196 mL	1.0979 mL	2.1959 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.5 mg/mL (5.49 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.49 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.49 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

AEP-IN-3 (compound 18) is an orally active, potent and brain penetrant asparagine endopeptidase (AEP) inhibitor, with an IC_{50} of 7.8 ± 0.9 nM. AEP-IN-3 can be used for Alzheimer's Disease (AD) research[1].

In Vivo

AEP-IN-3 (compound 18) has a bioavailability of 83% and a $T_{1/2}$[1].

AEP-IN-3 (20 mg/kg, orally, BID, for 5 days) shows significantly inhibited activity of AEP in brain in TauP301L transgenic mice [1].

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

Animal Model:	Mice producing the 2N4R isoform of human Tau containing the P301L mutation in aFVB/N genetic background (3.8 months old)[1]
Dosage:	20 mg/kg
Administration:	Orally, BID with an interval of 7-8 h between doses for 5 days
Result:	Showed significantly inhibited activity of AEP in brain, reduced formation of the Tau N368 fragment. The effect on total Tau is not significant.

REFERENCES

[1]. Krummenacher D, et al. Discovery of Orally Available and Brain Penetrant AEP Inhibitors. J Med Chem. 2023 Dec 28;66(24):17026-17043.

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