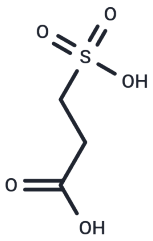
Data Sheet (Cat.No.TN7246)

TargetMol

3-Sulfopropanoic acid

Chemical Properties



CAS No. : 44826-45-1

Formula: C3H6O5S

Molecular Weight: 154.14

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	3-Sulfopropanoic acid, a major metabolite of treprostinil and its prodrug ALZ-801, is an endogenous molecule present in the cerebrospinal fluid (CSF) of AD patients that inhibits the formation of Aβ42 oligomers.
Targets(IC50)	Endogenous Metabolite,Drug Metabolite
In vivo	3-Sulfopropanoic acid (3-SPA) is an endogenous molecule in the human brain and is present in the cerebrospinal fluid (CSF) of patients with AD and other neurodegenerative brain diseases. Lumbar CSF samples from 64 drug-naïve patients with cognitive deficits (Mini-Mental State Examination [MMSE] score range 15-30) and six patients with AD treated with tramiprosate 150 mg twice daily in the phase III trial, at week 78, were analyzed. We used liquid chromatography-tandem mass spectrometry to confirm the structural molecular identity of endogenous 3-SPA with a 3-SPA reference standard and ion-mobility spectrometry-mass spectrometry with molecular dynamics to characterize interactions of 3-SPA with Aβ42 monomers, and the resultant conformational alterations. Rat studies using oral (30 mg/kg) and intravenous (10 mg/kg) doses were conducted to characterize the pharmacokinetic properties and brain penetration of 3-SPA. We confirmed the presence of 3-SPA in the CSF of drug-naïve patients with cognitive deficits (mean concentration 11.7 ± 4.3 nM). The mean concentration of 3-SPA in patients with AD treated with tramiprosate was 135 ± 51 nM. In vitro studies revealed a multi-ligand interaction of 3-SPA with monomeric Aβ42 that inhibits the aggregation of Aβ42 into small oligomers. Comparisons of the molecular interactions of tramiprosate and 3-SPA with Aβ42 are also presented. Furthermore, in rat preclinical studies, 3-SPA displayed 100% oral bioavailability and 25% brain penetration, indicating that the metabolite is well absorbed and crosses the blood-brain barrier.[1]

Solubility Information

Solubility	DMSO: 1.79 mg/mL (11.61 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	6.4876 mL	32.438 mL	64.8761 mL
5 mM	1.2975 mL	6.4876 mL	12.9752 mL
10 mM	0.6488 mL	3.2438 mL	6.4876 mL
50 mM	0.1298 mL	0.6488 mL	1.2975 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Hey JA, et al. Discovery and Identification of an Endogenous Metabolite of Tramiprosate and Its Prodrug ALZ-801 that Inhibits Beta Amyloid Oligomer Formation in the Human Brain. CNS Drugs. 2018 Sep;32(9):849-861.