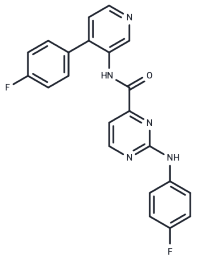
Data Sheet (Cat.No.T77341)

TargetMol
YOUR TARGET MOLECULES

GSK-3 inhibitor 4

Chemical Properties



CAS No. : 2227279-83-4

Formula: C22H15F2N5O

Molecular Weight: 403.38

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	GSK-3 inhibitor 4 is an orally active and brain-permeable triple inhibitor of GSK-3, CDK2 and CDK5 with inhibitory effects on GSK-3β, GSK-3α, CDK2 and CDK5, with IC50 values of 0.56 nM, 0.45 nM, 0.47 μM, 0.68 μM, respectively.GSK-3 inhibitor 4 can effectively reduce Tau protein levels. GSK-3 inhibitor 4 can effectively reduce the level of Tau protein.GSK-3 inhibitor 4 can be used in the study of Alzheimer's disease.
Targets(IC50)	GSK-3,CDK
In vitro	GSK-3 inhibitor 4 (compound 40) is effective against CDK2 (840-fold, IC50 = 0.47 μM), CDK5 (1200-fold, IC50 = 0.68 μM), GSK-3β (IC50 = 0.56 nM), and GSK-3α (IC50 = 0.45 nM) exhibits excellent selectivity.[1] GSK-3 inhibitor 4 has good permeability and shows a high ability to bind to plasma proteins and brain tissue due to its lipophilicity.[1]
In vivo	GSK-3 inhibitor 4 (10 mg/kg; p.o.) reduced pTau396 by 37% when the nanosuspension was administered orally at a dose of 10 mg/kg.[1] GSK-3 inhibitor 4 (2 mg/kg, i.v.; 10 mg/kg, p.o.) exhibits low-moderate clearance, ranging from 15.8 to 23.3 mL/min/kg, and is well absorbed when administered orally as a solution.[1]

Solubility Information

Solubility	DMSO: 50 mg/mL (123.95 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4791 mL	12.3953 mL	24.7905 mL
5 mM	0.4958 mL	2.4791 mL	4.9581 mL
10 mM	0.2479 mL	1.2395 mL	2.4791 mL
50 mM	0.0496 mL	0.2479 mL	0.4958 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.

Reference

Hartz RA, et al. Discovery of 2-(Anilino)pyrimidine-4-carboxamides as Highly Potent, Selective, and Orally Active Glycogen Synthase Kinase-3 (GSK-3) Inhibitors. J Med Chem. 2023 Jun 8;66(11):7534-7552.