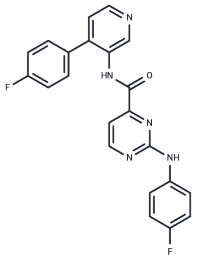
Data Sheet (Cat.No.T77341)

TargetMol

GSK-3 inhibitor 4

Chemical Properties



CAS No. : 2227279-83-4

Formula: C22H15F2N5O

Molecular Weight: 403.38

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	GSK-3 inhibitor 4 is an orally active and brain-permeable compound that acts as a triple inhibitor of GSK-3, CDK2, and CDK5, with IC50 values of 0.56 nM (GSK-3β), 0.45 nM (GSK-3α), 0.47 μM (CDK2), and 0.68 μM (CDK5). It effectively reduces Tau protein levels and can be used in the study of Alzheimer's disease.
Targets(IC50)	CDK,GSK-3
In vitro	GSK-3 inhibitor 4 (compound 40) demonstrates excellent selectivity and efficacy 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). It also exhibits good permeability and a high capacity for binding 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 administered orally as a nanosuspension. GSK-3 inhibitor 4 (2 mg/kg, i.v.; 10 mg/kg, p.o.) exhibits low to moderate clearance (15.8 to 23.3 mL/min/kg) and is well absorbed orally in solution.[1]

Solubility Information

Solubility	DMSO: 50 mg/mL (123.95 mM),Sonication is recommended. (< 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.

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

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.