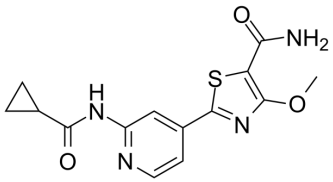
GSK-3β inhibitor 2

Cat. No.:	HY-130795
CAS No.:	1702428-31-6
Molecular Formula:	$C_{14}H_{14}N_4O_3S$
Molecular Weight:	318.35
Target:	GSK-3
Pathway:	PI3K/Akt/mTOR; Stem Cell/Wnt
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 : 5 mg/mL (15.71 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.1412 mL	15.7060 mL	31.4120 mL
	5 mM	0.6282 mL	3.1412 mL	6.2824 mL
	10 mM	0.3141 mL	1.5706 mL	3.1412 mL

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

BIOLOGICAL ACTIVITY

Description

GSK-3β inhibitor 2 (Compound 3) is a potent, selective and orally active GSK-3β inhibitor with an IC_{50} of 1.1 nM. GSK-3β inhibitor 2 can cross the blood-brain barrier. GSK-3β inhibitor 2 has the potential for Alzheimer's disease[1].

IC_{50} & Target

GSK-3β
1.1 nM (IC_{50})

In Vitro

The pyridine carboxamide of GSK-3β inhibitor 2 (Compound 3) makes hydrogen bonds with the hinge V135 backbone amide, and the carbonyl oxygen of the thiazolyl primary amide formed a critical hydrogen bond with K85. The quality of the electron density for the methyl group of the methoxy moiety in GSK-3β inhibitor 2 does not allow its unambiguous placement in the model, but a small molecule crystal structure of GSK-3β inhibitor 2 determined by single crystal X-ray diffraction method confirmed the intramolecular hydrogen bonding between the methoxy -O- and the amide N-H in GSK-3β inhibitor 2[1].

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

In Vivo

The elevation of hyperphosphorylated Tau (pTau) is mimicked in LaFerla 3xTg-C57BL6 mice, and accordingly, these mice are

	used as an in vivo model of Alzheimer's disease. GSK-3β inhibitor 2 (Compound 3) shows a significant reduction in pTau396 when administered orally at 30 mg/kg as a nanosuspension to LaFerla 3xTg-C57BL6 male mice. GSK-3β inhibitor 2 shows only modest brain exposure (B/P = 0.26) as determined as a single time point[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Sivaprakasam P, et al. Discovery of new acylaminopyridines as GSK-3 inhibitors by a structure guided in-depth exploration of chemical space around a pyrrolopyridinone core. Bioorg Med Chem Lett. 2015 May 1;25(9):1856-63.

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