BMS-986176

Cat. No.: HY-134829

CAS No.: 1815613-42-3

Molecular Formula: $C_{19}H_{23}F_4N_3O$

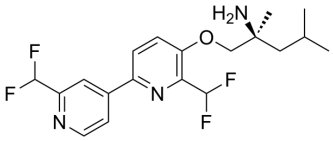
Molecular Weight: 385.4

Target: AAK1

Pathway: Neuronal Signaling

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 220 mg/mL (570.84 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5947 mL	12.9735 mL	25.9471 mL
	5 mM	0.5189 mL	2.5947 mL	5.1894 mL
	10 mM	0.2595 mL	1.2974 mL	2.5947 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 5.5 mg/mL (14.27 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 5 mg/mL (12.97 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (12.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BMS-986176 (LX-9211) is a highly selective, brain-penetrant, potent AAK1 (adaptor associated kinase 1) inhibitor with an IC_{50} of 2 nM. BMS-986176 can be used for neurodegenerative diseases research[1].

IC_{50} & Target

IC50: 2 nM (AAK1)[1]

In Vitro

Adaptor associated kinase 1 (AAK1) is a member of the Arkl/Prkl family of serine/threonine kinases. AAKl mRNA exists in two splice forms termed short and long. The long form predominates and is highly expressed in brain and heart. AAKl is enriched in synaptosomal preparations and is co-localized with endocytic structures in cultured cells. AAKl modulates clatherin coated endocytosis, a process that is important in synaptic vesicle recycling and receptor-mediated endocytosis[1].

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

REFERENCES

[1]. Guanglin Luo, et al. Biaryl kinase inhibitors. WO2015153720A1.

[2]. Guanglin Luo, et al. Discovery of (S)-1-((2',6-Bis(difluoromethyl)-[2,4'-bipyridin]-5-yl)oxy)-2,4-dimethylpentan-2-amine (BMS-986176/LX-9211): A Highly Selective, CNS Penetrable, and Orally Active Adaptor Protein-2 Associated Kinase 1 Inhibitor in Clinical Trials for the Treatment of Neuropathic Pain. J Med Chem. 2022 Mar 24;65(6):4457-4480.

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