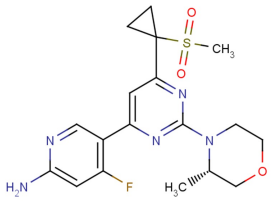
Data Sheet (Cat.No.T12460)

TargetMol
A DRUG SCREENING EXPERT

PI3K/mTOR Inhibitor-1

Chemical Properties



CAS No.:	1949802-49-6
Formula:	C18H22FN5O3S
Molecular Weight:	407.46
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	PI3K/mTOR Inhibitor-1 is a potent, orally bioavailable dual inhibitor of PI3K/mTOR (PI3Kα/PI3Kβ/PI3Kδ/PI3Kγ/mTOR with IC50s of 20/376/204/46/186 nM)
Targets(IC_{50})	PI3Kα: 20 nM PI3Kβ: 376 nM PI3Kγ: 204 nM PI3Kδ: 46 nM mTOR: 186 nM
In vitro	PI3K/mTOR Inhibitor-1 (Compound 26) as a potent dual PI3K/mTOR inhibitor. It exhibited high inhibitory activity against PI3Kα/β/γ/δ (IC50 = 20/376/204/46 nM) and mTOR (IC50 = 189 nM), potent functional suppression of AKT phosphorylation (IC50 = 196 nM), and excellent antiproliferative effects on a panel of cancer cells. Enzymic data and modeling simulation indicate that a cyclopropyl ring on the C4 sulfone chain and a fluorine on the C6 aminopyridyl moiety are responsible for its maintained PI3K activity and enhanced mTOR potency, respectively.
In vivo	PI3K/mTOR Inhibitor-1 (Compound 26) exhibited higher efficiency(antiproliferative effects) in the HT-29 colorectal carcinoma xenograft model at the daily dose of 3.75 and 7.5 mg/kg relative to BKM120 at the dose of 15 and 30 mg/kg.

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.454 mL	12.271 mL	24.542 mL
5 mM	0.491 mL	2.454 mL	4.908 mL
10 mM	0.245 mL	1.227 mL	2.454 mL
50 mM	0.049 mL	0.245 mL	0.491 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Shen S, et al. Discovery of an Orally Bioavailable Dual PI3K/mTOR Inhibitor Based on Sulfonyl-Substituted Morpholinopyrimidines. ACS Med Chem Lett. 2018 Jun 25;9(7):719-724.

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