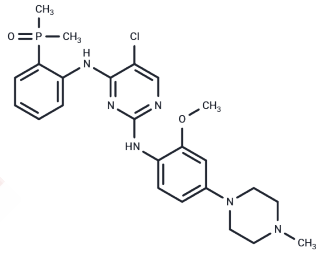
Data Sheet (Cat.No.T38584)

TargetMol

ALK-IN-12

Chemical Properties



CAS No. : 1197958-53-4

Formula: C24H30ClN6O2P

Molecular Weight: 500.97

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	ALK-IN-12 is a highly potent and orally active inhibitor of anaplastic lymphoma kinase (ALK), demonstrating an exceptional IC50 value of 0.18 nM. Additionally, ALK-IN-12 displays inhibitory activity against insulin-like growth factor 1 receptor (IGF1R) and insulin receptor (InsR), with IC50 values of 20.3 nM and 90.6 nM, respectively. Notably, its antitumor effects have been observed, making it a promising compound for targeted cancer therapy.
Targets(IC50)	Others,ALK
In vitro	ALK-IN-12 (compound 11e) effectively reduces the viability of the Karpas-299 ALCL cell line with an inhibition concentration (IC50) of 28.3 nM[1].
In vivo	Administered orally at doses ranging from 10-50 mg/kg daily for 13 consecutive days, ALK-IN-12 exhibited dose-dependent antitumor activity in a study involving 8-10 week old female SCID/beige mice hosting Karpas-299 xenografts expressing NPM-ALK fusion, achieving tumor stasis at the highest dose of 50 mg/kg. Intravenously given to 6-8 week old female CD rats at 3 mg/kg, ALK-IN-12 displayed pharmacokinetic parameters with an area under the curve (AUC) from time zero to infinity of 3039 ng·h/mL, a clearance (CL) rate of 0.91 h/kg, a half-life (t 1/2) of 6.6 hours, and a steady-state volume of distribution (V ss) of 6.12 L/kg. Similarly, when administered orally at 10 mg/kg to 6-8 week old female CD rats, it showed a maximum concentration (C max) of 3254 ng/mL, an AUC from time zero to infinity of 4056 ng·h/mL, time to reach maximum concentration (t max) of 6.0 hours, a half-life of 12.5 hours, and a bioavailability (F) of 39%.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9961 mL	9.9806 mL	19.9613 mL
5 mM	0.3992 mL	1.9961 mL	3.9923 mL
10 mM	0.1996 mL	0.9981 mL	1.9961 mL
50 mM	0.0399 mL	0.1996 mL	0.3992 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

Huang WS, et al. Discovery of Brigatinib (AP26113), a Phosphine Oxide-Containing, Potent, Orally Active Inhibitor of Anaplastic Lymphoma Kinase. J Med Chem. 2016;59(10):4948-4964.