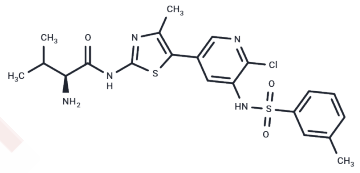
Data Sheet (Cat.No.T10804)

TargetMol

CHMFL-PI3KD-317

Chemical Properties



CAS No. : 2244992-76-3

Formula: C21H24ClN5O3S2

Molecular Weight: 494.03

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	CHMFL-PI3KD-317 is a highly potent, selective, and orally active PI3Kδ inhibitor with an IC50 of 6 nM, exhibiting over 10-1500 fold selectivity over other class I, II, and III PIKK family isoforms, such as PI3Kα (IC50, 62.6 nM), PI3Kβ (IC50, 284 nM), PI3Kγ (IC50, 202.7 nM), PIK3C2A (IC50, >10000 nM), PIK3C2B (IC50, 882.3 nM), VPS34 (IC50, 1801.7 nM), PI4KIIIA (IC50, 574.1 nM), and PI4KIIIB (IC50, 300.2 nM). It inhibits PI3Kδ-mediated Akt T308 phosphorylation in Raji cells with an EC50 of 4.3 nM and has antiproliferative effects on cancer cells.
Targets(IC50)	PI3K,PI4K
In vitro	CHMFL-PI3KD-317 exhibits over 10-1500 fold selectivity over other class I, II and III PIKK family isoforms, such as PI3Kα (IC50, 62.6 nM), PI3Kβ (IC50, 284 nM), PI3Kγ (IC50, 202.7 nM), PIK3C2A (IC50, >10000 nM), PIK3C2B (IC50, 882.3 nM), PI4KIIIA (IC50, 574.1 nM) and PI4KIIIB (IC50, 300.2 nM). CHMFL-PI3KD-317 has antiproliferative effects, with GI50s of 4.0, 3.5, 4.8, 3.0, 3.3 μM against NALM-6, PF382, MV4-11, MOLM-13 cells, and MOLM-14, respectively.
In vivo	CHMFL-PI3KD-317 (Compound 15i; 25, 50, and 100mg/kg/day, p.o., for 14 days) inhibits the growth of the MOLM14 tumor in mice and, in Sprague-Dawley rats, shows favorable oral bioavailability and an acceptable half-life (T1/2=3.28h).

Solubility Information

Solubility	DMSO: 45 mg/mL (91.09 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.05 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0242 mL	10.1208 mL	20.2417 mL
5 mM	0.4048 mL	2.0242 mL	4.0483 mL
10 mM	0.2024 mL	1.0121 mL	2.0242 mL
50 mM	0.0405 mL	0.2024 mL	0.4048 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

Liang X, et al. Discovery of (S)-2-amino-N-(5-(6-chloro-5-(3-methylphenylsulfonamido)pyridin-3-yl)-4-methylthiazol-2-yl)-3-methylbutanamide (CHMFL-PI3KD-317) as a potent and selective phosphoinositide 3-kinase delta (PI3Kδ) inhibitor. Eur J Med Chem. 2018 Aug 5;156:831-846.