Theliatinib

Cat. No.: HY-104066

CAS No.: 1353644-70-8

Molecular Formula: $C_{25}H_{26}N_6O_2$

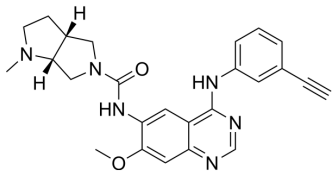
Molecular Weight: 442.51

Target: EGFR

Pathway: JAK/STAT Signaling; Protein Tyrosine Kinase/RTK

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 5 mg/mL (11.30 mM; Need ultrasonic)

DMSO : 1 mg/mL (2.26 mM; ultrasonic and warming and adjust pH to 3 with HCl and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2598 mL	11.2992 mL	22.5984 mL
5 mM	0.4520 mL	2.2598 mL	4.5197 mL
10 mM	0.2260 mL	1.1299 mL	2.2598 mL

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

BIOLOGICAL ACTIVITY

Description

Theliatinib (Xiliertinib) is a potent, ATP-competitive, orally active and highly selective EGFR inhibitor with a K_i of 0.05 nM and an IC_{50} of 3 nM. Theliatinib has an IC_{50} of 22 nM for EGFR T790M/L858R mutant. Theliatinib shows >50-fold selectivity for EGFR than other kinases[1]. Theliatinib is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

EGFR 3 nM (IC_{50})	EGFR 0.05 nM (Ki)	EGFR (L858R/T790M) 22 nM (IC_{50})

In Vitro

Theliatinib significantly inhibits EGFR phosphorylation in A431 cells with an IC_{50} of 7 nM. Theliatinib also inhibits A431, H292 and FaDu cells survival with IC_{50} values of 80 nM, 58 nM and 354 nM, respectively[1].

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

In Vivo

Theliatinib (2-15 mg/kg; oral administration;daily; for 21 days; NOD-SCID mice; PDECX 1T0950 model) treatment demonstrates tumor regression of 75% at the end of study, and with a dose response[1].

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

Animal Model:	NOD-SCID mice injected with esophageal cancer cells (PDECX 1T0950 model)[1]
Dosage:	2 mg/kg, 5 mg/kg, 15 mg/kg
Administration:	Oral administration;daily; for 21 days
Result:	Attenuated tumor growth in PDECX 1T0950 model in a dose-dependent manner.

REFERENCES

[1]. Ren Y, et al. Anti-tumor efficacy of theliatinib in esophageal cancer patient-derived xenografts models with epidermal growth factor receptor (EGFR) overexpression and gene amplification. Oncotarget. 2017 Apr 19;8(31):50832-50844.

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