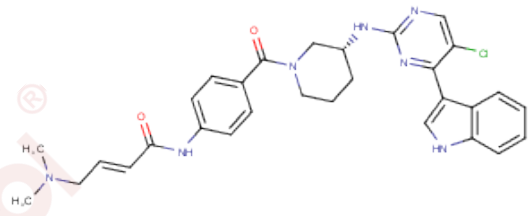
Data Sheet (Cat.No.T4293)

TargetMol
A DRUG SCREENING EXPERT

THZ531

Chemical Properties



CAS No. : 1702809-17-3

Formula: C30H32ClN7O2

Molecular Weight: 558.08

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	THZ531 is a covalent inhibitor of both CDK12(IC50=158 nM) and CDK13(IC50=69 nM).
Targets(IC50)	CDK
In vitro	In Jurkat cell, THZ531(IC50=50 nM) treatment leads to a dramatic and irreversible decrease proliferation.THZ531 potently inhibits CDK12(IC50=158 nM) and CDK13 (IC50=69 nM).
Kinase Assay	Cells are treated with THZ531 for 6 hours.After treatment cells are washed 2-fold with cold PBS and then lysed in the following lysis buffer: Hepes(50 mM, pH 7.4), NaCl（150 mM）, 1% Nonidet P40 substitute, EDTA（5 mM）, DTT（1 mM）, and protease/phosphatase cocktails.Lysates are treated with bio-THZ1 or bio-TH531 for pulldown overnight at 4°C.
Cell Research	Jurkat cells are plated in 96-well plates at 20,000 cells/well in fresh media and treated with THZ531 or DMSO at the indicated concentrations for 72 hours. HAP1 cells are seeded in 96-well plates at 12,000 cells/well in fresh media and 24 hours later are treated with THZ531 at the indicated concentrations for 72 hours. Anti-proliferative effect of THZ531 is assessed. To assess the effect of inhibitor washout on anti-proliferation of Jurkat cells, cells are treated with THZ531 or DMSO for 6 hrs. Inhibitor-containing medium is then removed and incubated with or without THZ531 for 66 hrs. Anti-proliferative effect of THZ531 is assessed. All proliferation assays are performed in biological triplicate. IC50s are determined using non-linear regression curve fit.

Solubility Information

Solubility	DMSO: 45 mg/mL (80.63 mM), (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.7919 mL	8.9593 mL	17.9186 mL
5 mM	0.3584 mL	1.7919 mL	3.5837 mL
10 mM	0.1792 mL	0.8959 mL	1.7919 mL
50 mM	0.0358 mL	0.1792 mL	0.3584 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.

Reference

Zhang G M, Huang S S, Ye L X, et al. Reciprocal positive regulation between BRD4 and YAP in GNAQ-mutant uveal melanoma cells confers sensitivity to BET inhibitors. Pharmacological Research. 2022: 106464.