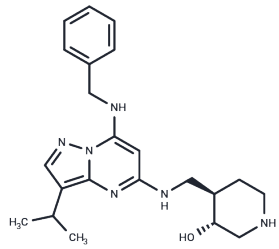
Data Sheet (Cat.No.T10898)

TargetMol

Samuraciclib hydrochloride

Chemical Properties



CAS No. : 1805789-54-1

Formula: C22H31ClN6O

Molecular Weight: 430.97

Storage: Store at low temperature,Keep away from moisture
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	Samuraciclib hydrochloride (ICEC0942 hydrochloride) is a potent, selective, ATP competitive and oral active CDK7 inhibitor with IC50 of 41 nM. The selectivity of Samuraciclib hydrochloride is 45-, 15-, 230- and 30-fold higher than CDK1, CDK2 (IC50 is 578 nM), CDK5 and CDK9 respectively. Samuraciclib hydrochloride inhibits the growth of breast cancer cell lines with GI50 values between 0.2-0.3 μM. Samuraciclib hydrochloride has anti-tumor effects.
Targets(IC50)	Apoptosis,CDK
In vitro	Samuraciclib (ICEC0942; 0-10 μM; 24 hours; HCT116 cells) treatment can promote apoptosis. Samuraciclib (ICEC0942; 0-10 μM; 24 hours; HCT116 cells) treatment can induce cell cycle arrest. Samuraciclib (ICEC0942; 0-10 μM; 0-24 hours; HCT116 cells) treatment inhibited the phosphorylation of PolII CTD in HCT116 colon cancer cells in a dose- and time-dependent manner. ICEC0942 also inhibits the phosphorylation of CDK1, CDK2 and retinoblastoma. Samuraciclib (ICEC0942) inhibits the growth of MCF7, T47D, MDA-MB-231, HS578T, MDA-MB-468, MCF10A and HMEC cells with GI50 values of 0.18 μM, 0.32 μM, 0.33 μM, 0.21 μM, 0.22 μM It is 0.67 μM and 1.25 μM.
In vivo	Samuraciclib (ICEC0942; 100 mg / kg; oral tube; daily; 14 consecutive days; female nu / nu-BALB / c athymic nude mice) treatment inhibited tumor growth by 60% on day 14 with a significant reduction in PolII Ser2 and Ser5 phosphorylation in PBMC and tumors. The combination of Samuraciclib (ICEC0942) and ICI 47699 treatment showed complete stagnation of estrogen receptor (ER) positive tumor xenografts.

Solubility Information

Solubility	H2O: 55 mg/mL (127.62 mM),Sonication is recommended. DMSO: 150 mg/mL (348.05 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: 10 mg/mL (23.2 mM),Solution. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.64 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*

In vivo Formulation	*vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.3203 mL	11.6017 mL	23.2035 mL
5 mM	0.4641 mL	2.3203 mL	4.6407 mL
10 mM	0.232 mL	1.1602 mL	2.3203 mL
50 mM	0.0464 mL	0.232 mL	0.4641 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

Patel H, et al. ICEC0942, an Orally Bioavailable Selective Inhibitor of CDK7 for Cancer Treatment. Mol Cancer Ther. 2018 Jun;17(6):1156-1166.
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.
Hazel P, et al. Inhibitor Selectivity for Cyclin-Dependent Kinase7: AStructural, Thermodynamic, and Modelling Study. ChemMedChem. 2017 Mar 7;12(5):372-380.