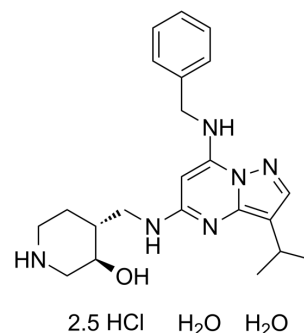


Samuraciclib hydrochloride hydrate

Cat. No.: HY-103712B
Molecular Formula: $C_{22}H_{30}N_6O \cdot (2.5HCl) \cdot (2H_2O)$
Molecular Weight: 521.7
Target: CDK; Apoptosis
Pathway: Cell Cycle/DNA Damage; Apoptosis
Storage: 4°C, stored under nitrogen, away from moisture
 * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen, away from moisture)



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (191.68 mM; Need ultrasonic)					
	Preparing Stock Solutions	<div>Solvent Concentration</div>	Mass	1 mg	5 mg	10 mg
		1 mM	1.9168 mL	9.5841 mL	19.1681 mL	
		5 mM	0.3834 mL	1.9168 mL	3.8336 mL	
		10 mM	0.1917 mL	0.9584 mL	1.9168 mL	
Please refer to the solubility information to select the appropriate solvent.						
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (4.79 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (4.79 mM); Clear solution					
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: 2.5 mg/mL (4.79 mM); Suspended solution; Need ultrasonic					

BIOLOGICAL ACTIVITY

Description	Samuraciclib (CT7001) hydrochloride hydrate is a potent, selective, ATP-competitive and orally active CDK7 inhibitor, with an IC ₅₀ of 41 nM. Samuraciclib hydrochloride hydrate displays 45-, 15-, 230- and 30-fold selectivity over CDK1, CDK2 (IC ₅₀ of 578 nM), CDK5 and CDK9, respectively. Samuraciclib hydrochloride hydrate inhibits the growth of breast cancer cell lines with GI ₅₀ values between 0.2-0.3 μM. Samuraciclib hydrochloride hydrate has anti-tumor effects ^{[1][2]} .			
IC ₅₀ & Target	CDK7 41 nM (IC ₅₀)	CDK2 578 nM (IC ₅₀)	CDK1 1.8 μM (IC ₅₀)	CDK4 49 μM (IC ₅₀)
	CDK5	CDK6	CDK9	

	9.4 μM (IC ₅₀)	31 μM (IC ₅₀)	1.2 μM (IC ₅₀)
In Vitro	Samuraciclib hydrochloride hydrate (ICEC0942; 0-10 μM; 24 hours; HCT116 cells) treatment promotes cell apoptosis ^[1] . Samuraciclib hydrochloride hydrate (ICEC0942; 0-10 μM; 24 hours; HCT116 cells) treatment induces cell cycle arrest ^[1] . Samuraciclib hydrochloride hydrate (ICEC0942; 0-10 μM; 0-24 hours; HCT116 cells) treatment inhibits the phosphorylation of PolII CTD in a dose and time dependent manner in HCT116 colon cancer cells. Samuraciclib trihydrochloride also inhibits phosphorylation of CDK1, CDK2 and retinoblastoma ^[1] . Samuraciclib (ICEC0942) hydrochloride hydrate inhibits the growth of MCF7, T47D, MDA-MB-231, HS578T, MDA-MB-468, MCF10A and HMEC cells with GI ₅₀ values of 0.18 μM, 0.32 μM, 0.33 μM, 0.21 μM, 0.22 μM, 0.67 μM and 1.25 μM, respectively ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
	Apoptosis Analysis ^[1]		
	Cell Line:	HCT116 cells	
	Concentration:	0 μM, 0.1 μM, 1 μM and 10 μM	
	Incubation Time:	24 hours	
	Result:	Induced caspase 3/7 and demonstrated PARP cleavage.	
	Cell Cycle Analysis ^[1]		
	Cell Line:	HCT116 cells	
	Concentration:	0 μM, 0.01 μM, 0.1 μM, 1 μM and 10 μM	
	Incubation Time:	24 hours	
	Result:	Showed accumulation of cells in G2/M.	
	Western Blot Analysis ^[1]		
	Cell Line:	HCT116 cells	
	Concentration:	0 μM, 0.01 μM, 0.1 μM, 1 μM and 10 μM	
	Incubation Time:	0 hour, 4 hours, 8 hours, 16 hours or 24 hours	
Result:	PolII CTD phosphorylation was inhibited in a dose and time dependent manner in HCT116 colon cancer cells.		
In Vivo	Samuraciclib (ICEC0942; 100 mg/kg; oral gavage; daily; for 14 days; female nu/nu-BALB/c athymic nude mice) hydrochloride hydrate treatment inhibits tumor growth by 60% at day 14, and is accompanied by highly significant reductions in PolII Ser2 and Ser5 phosphorylation in PBMCs and in tumors ^[1] . The combination of Samuraciclib (ICEC0942) hydrochloride hydrate and ICI 47699 treatment shows complete growth arrest of estrogen receptor (ER)-positive tumor xenografts ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
	Animal Model:	Female nu/nu-BALB/c athymic nude mice (7-week old) with MCF7 cells ^[1]	
	Dosage:	100 mg/kg	
	Administration:	Oral gavage; daily; for 14 days	
	Result:	At day 14, tumor growth was inhibited by 60%.	

CUSTOMER VALIDATION

- Proc Natl Acad Sci U S A. 2019 Jun 25;116(26):12986-12995.
- Cell Death Dis. 2019 Aug 9;10(8):602.
- Int J Mol Sci. 2022 Feb 24;23(5):2493.
- J Cancer Res Clin Oncol. 2022 Nov 18.

See more customer validations on www.MedChemExpress.com

REFERENCES

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

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA