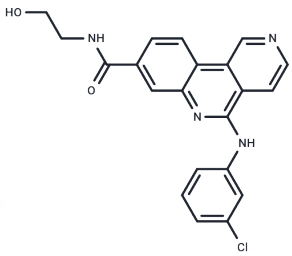
Data Sheet (Cat.No.T35557)

TargetMol

CK2 inhibitor 2

Chemical Properties



CAS No. : 2641079-92-5

Formula: C21H17ClN4O2

Molecular Weight: 392.84

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	CK2 Inhibitor 2, characterized as a potent, selective, and orally active inhibitor of CK2, demonstrates an impressive IC50 value of 0.66 nM. It exhibits high selectivity towards Clk2 with an IC50 of 32.69 nM in comparison to CK2. Furthermore, CK2 Inhibitor 2 has been shown to possess promising antiproliferative and antitumor activities [1].
Targets(IC50)	Casein Kinase
In vitro	CK2 inhibitor 2 (compound 1c) effectively inhibits the proliferation of PC-3, HCT-116, MCF-7, HT-29, T24, and LO2 cancer cell lines with IC50 values of 4.53 μM, 3.07 μM, 7.50 μM, 5.18 μM, 6.10 μM, and 96.68 μM, respectively. It induces dose-dependent apoptosis in HCT-116 cells, achieving a 55% apoptotic ratio at 20 μM after 24 hours. The compound reduces phosphorylated Akt1 S129 and Cdc37 S13 expression, suggesting suppression of survival pathways. It also inhibits ALDH1A1 enzyme activity (IC50 of 0.10 μM) and downregulates its transcription and protein expression in HCT-116 cells, indicating potential for targeting cancer-specific metabolic pathways.
In vivo	Administering CK2 inhibitor 2 at doses ranging from 60 to 90 mg/kg orally, twice daily for four weeks, significantly inhibits tumor growth in a dose-dependent manner, achieving a peak inhibition rate of 69% at the 90 mg/kg dosage. A single oral dose of 25 mg/kg in Sprague-Dawley rats reveals pharmacokinetic parameters such as a maximum concentration (C max) of 7017.8 ng/mL, an elimination half-life (t 1/2) of 6.67 hours, and a clearance rate (CL) of 0.60 L/h/kg. The study utilized male BALB/c athymic nude mice, aged 5 weeks and weighing 16-18 grams, injected with HCT-116 cells, demonstrating dose-dependent tumor growth inhibition without noticeable changes in body weight.

Solubility Information

Solubility	DMSO: 50 mg/mL (127.28 mM),Sonication and heating to 60°C are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 2.5 mg/mL (6.36 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	2.5456 mL	12.7278 mL	25.4557 mL
5 mM	0.5091 mL	2.5456 mL	5.0911 mL
10 mM	0.2546 mL	1.2728 mL	2.5456 mL
50 mM	0.0509 mL	0.2546 mL	0.5091 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

Wang Y, et, al. Discovery of 5-(3-Chlorophenylamino)benzo[c][2,6]naphthyridine Derivatives as Highly Selective CK2 Inhibitors with Potent Cancer Cell Stemness Inhibition. J Med Chem. 2021 Apr 22;64(8):5082-5098.