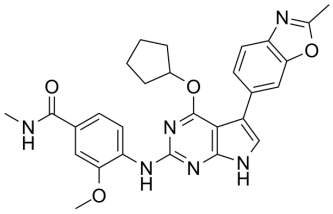
CC-671

Cat. No.:	HY-108709
CAS No.:	1618658-88-0
Molecular Formula:	$C_{28}H_{28}N_6O_4$
Molecular Weight:	512.56
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
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 : ≥ 60 mg/mL (117.06 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9510 mL	9.7550 mL	19.5099 mL
	5 mM	0.3902 mL	1.9510 mL	3.9020 mL
	10 mM	0.1951 mL	0.9755 mL	1.9510 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: ≥ 2.08 mg/mL (4.06 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.06 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.08 mg/mL (4.06 mM); Clear solution; Need warming

BIOLOGICAL ACTIVITY

Description

CC-671 is a dual TTK protein kinase/CDC2-like kinase (CLK2) inhibitor with IC_{50}s of 0.005 and 0.006 μM for TTK and CLK2, respectively.

IC_{50} & Target

CLK2
0.006 μM (IC_{50})

In Vitro	CC-671 (compound 23) is a dual TTK protein kinase/CDC2-like kinase (CLK2) inhibitor with IC_{50}s of 0.005 and 0.006 μM for TTK and CLK2, respectively. HCT-116 cell lysates treated with CC-671 at 3 μM for 1 h demonstrates that only four kinases show cellular binding of 75% or more including CLK2, CAMKK2, PIP4K22, and JNK[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	CC-671 (compound 23) demonstrates significant tumor growth inhibition (TGI) ((vehicle -treated/vehicle) ×100%) of 71% at both 10 and 20 mg/kg on a every 3 days (q3d) dosing schedule. The body weight loss (BWL) in the CC-671 treated group (20 mg/kg) is higher than in the 10 mg/kg group (17% vs 5%)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	The kinase selectivity profile of CC-671 (compound 23) is assessed. The screen is conducted with the concentration of CC-671 held constant at 3 μM. The TTK binding affinity is measured using the kinase binding assays. The kinase binding assays are based on the binding and displacement of a proprietary, Alexa Fluor 647-labeled, ATP-competitive kinase inhibitor scaffold[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Female SCID mice are inoculated subcutaneously with 5×10^6 Cal-51 cells. Mice with tumors of approximately 125 mm^3 are randomized and treated intravenously at various doses and schedules of CC-671 (compound 23) (n=8 to10/group). Tumors are measured twice a week for the duration of the study. The long and short axes of each tumor are measured using a digital caliper in millimeters and the tumor volumes are calculated[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cancer Cell. 2022 Sep 18;S1535-6108(22)00379-8.

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REFERENCES

[1]. Riggs JR, et al. The Discovery of a Dual TTK Protein Kinase/CDC2-Like Kinase (CLK2) Inhibitor for the Treatmentof Triple Negative Breast Cancer Initiated from a Phenotypic Screen. J Med Chem. 2017 Nov 9;60(21):8989-9002.

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