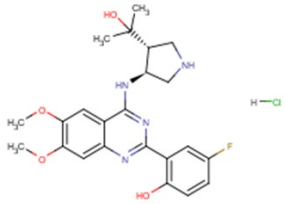
Data Sheet (Cat.No.T10718L)

TargetMol
A DRUG SCREENING EXPERT

CCT241533 hydrochloride

Chemical Properties



CAS No.:	1431697-96-9
Formula:	C23H28ClFN4O4
Molecular Weight:	478.94
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	CCT241533 hydrochloride is an effective and selective ATP competitive inhibitor of CHK2 (Ki: 1.16 nM; IC50: 3 nM).
Targets(IC_{50})	Chk2: 3 nM Chk1: 245 nM
In vitro	CCT241533 hydrochloride inhibits CHK2 (IC50: 3 nM) and shows minimal cross-reactivity against a panel of kinases at 1 μM. X-ray crystallography confirms that CCT241533 binds to CHK2 in the ATP pocket. CCT241533 blocks CHK2 activity in human tumor cell lines in response to DNA damage. CCT241533 does not potentiate the cytotoxicity of a selection of genotoxic agents in several cell lines. However, CCT241533 significantly potentiates the cytotoxicity of two structurally distinct PARP inhibitors. Clear induction of the pS516 CHK2 signal is seen with a PARP inhibitor alone and this activation is abolished by CCT241533. In HT-29, HeLa, and MCF-7, the cytotoxicity of CCT241533 (GI50) is 1.7, 2.2, and 5.1 μM, respectively [1]. CCT241533 hydrochloride is a potent CHK2 inhibitor (IC50: 3 nM), with selectivity (63-fold) over CHK1(IC50: 190 nM) and low hERG inhibition (IC50: 22 μM) [2].

Solubility Information

Solubility	DMSO: 100 mg/mL (208.79 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.088 mL	10.44 mL	20.879 mL
5 mM	0.418 mL	2.088 mL	4.176 mL
10 mM	0.209 mL	1.044 mL	2.088 mL
50 mM	0.042 mL	0.209 mL	0.418 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Anderson VE, et al. CCT241533 is a potent and selective inhibitor of CHK2 that potentiates the cytotoxicity of PARP inhibitors. Cancer Res. 2011 Jan 15;71(2):463-72.

2. Caldwell JJ, et al. Structure-based design of potent and selective 2-(quinazolin-2-yl)phenol inhibitors of checkpoint kinase 2. J Med Chem. 2011 Jan 27;54(2):580-90.

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