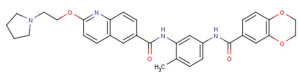
Data Sheet (Cat.No.T14905)

TargetMol
A DRUG SCREENING EXPERT

CCT251236

Chemical Properties



CAS No.:	1693731-40-6
Formula:	C32H32N4O5
Molecular Weight:	552.62
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	CCT251236 is an orally available Pirin ligand obtained from a heat shock transcription factor 1 (hsf1) phenotypic screen. It inhibits HSF1-mediated HSP72 induction (IC50: 19 nM).
Targets(IC_{50})	HSP72: 19 nM SK-OV-3 cells: None
In vitro	CCT367766 (0-100 nM; 24 hours) blocks 17-AAG induced he HSF1-mediated heat-shock proteins, HSP72, and HSP27 expression as a concentration manner in SK-OV-3 cells. CCT367766 blocks the induction of HSPA1A mRNA by 17-AAG in a dose-dependent manner. CCT367766 (0-100 nM; 24hours) displays the desired balance of in vitro properties while maintaining excellent cellular activity with a pIC50=7.73 ± 0.07 (IC50: 19 nM) for inhibition of HSF1-mediated HSP72 induction. The free GI50 is 1.1 nM in SK-OV-3 cells that calculated from the free fraction in the cell assay. CCT367766 (0-100 nM; 24 hours) pre-treated with 250 nM 17-AAG for 6h.
In vivo	CCT367766 (p.o.; 20 mg/kg; 33 days) has a clear therapeutic efficacy in mice with a tumor growth inhibition (%TGI) of 70% based on final tumor volumes. After 33 days, the mean tumor weights decrease 64% when compares to the control group. In addition, the compound's basicity and the high volume of the distribution shown in tumors with tumor concentrations of CCT367766 as high as 940 nM. CCT367766 (p.o.; 5 or 20 mg/kg) in nontumor bearing immunocompetent BALB/c mice exhibits free Cav0–24h value of 2.0 nM and 1.2 nM, respectively [2].

Solubility Information

Solubility	DMSO: 150 mg/mL (271.43 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.81 mL	9.048 mL	18.096 mL
5 mM	0.362 mL	1.81 mL	3.619 mL
10 mM	0.181 mL	0.905 mL	1.81 mL
50 mM	0.036 mL	0.181 mL	0.362 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. Cheeseman MD, et al. Discovery of a Chemical Probe Bisamide (CCT251236): An OrallyBioavailable Efficacious Pirin Ligand from a Heat ShockTranscription Factor 1 (HSF1) Phenotypic Screen. J Med Chem. 2017 Jan 12;60(1):180-201.

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