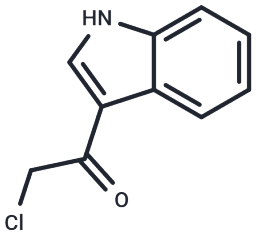
Data Sheet (Cat.No.T14034)

TargetMol

3CAI

Chemical Properties



CAS No. : 28755-03-5

Formula: C10H8ClNO

Molecular Weight: 193.63

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	3CAI is a potent and specific AKT1 and AKT2 inhibitor, demonstrating significant inhibition of AKT in an in vitro kinase assay. It suppressed the expression of AKT direct downstream targets (such as mTOR and GSK3β) and induced growth inhibition and apoptosis in colon cancer cells.
Targets(IC50)	Akt
In vitro	3CAI, a potential AKT inhibitor, exhibits significantly higher potency in inhibiting AKT1 compared to PI3K (60% inhibition at 1 μM vs 10 μM, respectively). In experiments with HCT116 and HT29 colon cancer cells treated with 3CAI (4 μM), I3C, or an AKT inhibitor in 1% FBS/McCoy's 5A (for HCT116) over four days, 3CAI notably increased apoptotic cell numbers versus untreated controls. Additionally, 3CAI markedly reduced AKT-mediated phosphorylation of mTOR (Ser2448) and GSK3β (Ser9) in a time-dependent manner, while also elevating pro-apoptotic proteins p53 and p21 after 12 or 24 hours of treatment. In vitro kinase assays revealed that 3CAI solely inhibits AKT1 kinase activity without affecting the activities of MEK1, JNK1, ERK1, and TOPK at 1 μM. Its capability to suppress AKT1 and AKT2 activities indicates a dose-dependent effect, with a profound impact on downstream AKT targets and the induction of apoptosis.
In vivo	To assess the in vivo antitumor efficacy of 3CAI, athymic nude mice with HCT116 cancer cell-induced tumors on their right flank were orally administered 3CAI at doses of 20 or 30 mg/kg, I3C at 100 mg/kg, or a vehicle control, five times weekly for a duration of 21 days. The higher dosage of 3CAI (30 mg/kg) was found to notably suppress the expression of AKT-target proteins in tumor tissues. Furthermore, this dosage significantly reduced tumor growth by 50% compared to the control group ($p<0.05$), without inducing noticeable side effects or substantial weight loss in the mice, suggesting a good tolerance to the treatment.

Solubility Information

Solubility	DMSO: 246 mg/mL (1270.46 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (25.82 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one.*

In vivo Formulation	*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	5.1645 mL	25.8224 mL	51.6449 mL
5 mM	1.0329 mL	5.1645 mL	10.329 mL
10 mM	0.5164 mL	2.5822 mL	5.1645 mL
50 mM	0.1033 mL	0.5164 mL	1.0329 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

Kim DJ, et al. (3-Chloroacetyl)-indole, a novel allosteric AKT inhibitor, suppresses colon cancer growth in vitro and in vivo. Cancer Prev Res (Phila). 2011 Nov;4(11):1842-51.