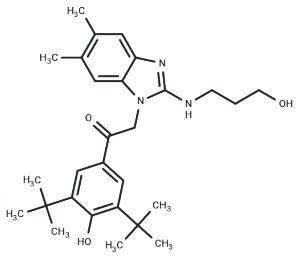
Data Sheet (Cat.No.TQ0305)

TargetMol

CID-2858522

Chemical Properties



CAS No. : 758679-97-9

Formula: C28H39N3O3

Molecular Weight: 465.63

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	CID-2858522 is an effective and specific antigen receptor-mediated NF-κB activation inhibitor (IC50: 70 nM).
Targets(IC50)	NF-κB
In vitro	CID-2858522 (Compound 1) also inhibits testosterone hydroxylase in the presence of human liver microsomes and an NADPH generating system (IC50: 85 μM) [1]. In the HEK293 cell line, CID-2858522 suppresses NF-κB reporter gene activity in a concentration-dependent manner, with IC50 ~70 nM and with maximum inhibition achieved at 0.25-0.5 μM. In contrast, CID-2858522 does not inhibit TNF-induced NF-κB-reporter gene activity at concentrations as high as 4 μM. CID-2858522 also potently inhibits PMA/Ionomycin-induced NF-κB reporter gene activity in transient transfection assays [2].
In vivo	CID-2858522 exhibits nonlinear pharmacokinetics, showing higher serum levels at the 0.5 h measurement time for the 30 mg/kg dose compared to 50 mg/kg but displaying typical dose-dependent behavior when measured at t=3 h. The increasing accumulation seen at a dose of 50 mg/kg may be due to a depot effect created by CYP3A4 inhibition. The cohort exhibits clear signs of morbidity at t=3 h at the 50 mg/kg dose [2].
Cell Research	Cell viability is estimated based on cellular ATP levels. HEK293 cells at a density of 10^5/mL are seeded at 90 μL per well in 96-well white plates and cultured overnight. Compounds (e.g., CID-2858522; 1 μM, 2 μM, 3 μM, and 4 μM) are added (5 μL in medium) to wells and cells are cultured for 16 h, Finally, 50 μL ATPlite solution is added to each well and luminescence activity is read using a luminometer [2].
Animal Research	Three male mice are subjected to CID-2858522 (single i.p doses at 10, 30, and 50 mg/kg). Blood is drawn at 0.5 and 3 h, and subsequent LC/MS analysis of pooled samples is performed to determine the overall blood levels of CID-2858522 [2].

Solubility Information

Solubility	DMSO: 6.5 mg/mL (13.96 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: 1 mg/mL (2.15 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	2.1476 mL	10.7381 mL	21.4763 mL
5 mM	0.4295 mL	2.1476 mL	4.2953 mL
10 mM	0.2148 mL	1.0738 mL	2.1476 mL
50 mM	0.043 mL	0.2148 mL	0.4295 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

Okolotowicz KJ, et al. Selective benzimidazole inhibitors of the antigen receptor-mediated NF-kappaB activationpathway. Bioorg Med Chem. 2010 Mar 1;18(5):1918-24.

Peddibhotla S, et al. Inhibition of protein kinase C-driven nuclear factor-kappaB activation: synthesis, structure-activity relationship, and pharmacological profiling of pathway specific benzimidazole probe molecules. J Med Chem. 2010 Jun 24;53(12):4793-7.