Data Sheet (Cat.No.TQ0305)

CID-2858522

Chemical Properties

CAS No.:	758679-97-9
Formula:	C28H39N3O3
Molecular Weight:	465.63
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	CID-2858522 is an effective and specific antigen receptor-mediated NF-κB activation inhibitor (IC50: 70 nM).
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: Soluble (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.148 mL	10.738 mL	21.476 mL
5 mM	0.43 mL	2.148 mL	4.295 mL
10 mM	0.215 mL	1.074 mL	2.148 mL
50 mM	0.043 mL	0.215 mL	0.43 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. 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.

2. 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.

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