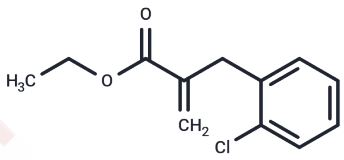
Data Sheet (Cat.No.T4217)

TargetMol

INF39

Chemical Properties



CAS No. : 866028-26-4

Formula: C12H13ClO2

Molecular Weight: 224.68

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	INF39 is a noncytotoxic and irreversible NLRP3 inhibitor.
Targets(IC50)	NOD-like Receptor (NLR),NOD
In vitro	INF39 possibly reacts with Cys-SH residues in the active site of cysteine protease caspase-1 but does not directly inhibit caspase-1 activity. INF39 (10 μM) can markedly inhibit ATP- and nigericin-induced IL-1β release. In the macrophages, INF39 suppresses caspase-1 activation and pyroptosis. INF39 can also block the NF-κB pathway. INF39 can reduce the steady-state (or basal) BRET signal of NLRP3, and not affect the viability of cells. INF39 cannot affect the initial conformational changes suffered by NLRP3 upon sensing the decrease of intracellular K+, but it affects the second step of NLRP3 conformational change. INF39 reaches the intestinal epithelium without undergoing chemical modifications. It is likely to act locally at the mucosal epithelial level after absorption into epithelial cells.
In vivo	INF39 (p.o.) reduces systemic and colonic inflammation in rats treated with 2,4-dinitrobenzene sulfonic acid. In inflamed rats, INF39 (12.5/25/50 mg/ kg) markedly increases body weight. DNBS causes a significant increment of spleen weight (+39.3%). This increase is markedly reduced by administration of INF39 (+2.2, +4.3 and +4.8% at 12.5, 25, 50 mg/kg, respectively). The inhibition of NLRP3 inflammasome complex with INF39 can dose-dependently attenuate the decrease in colonic length (?19, ?13 and ?8% at 12.5, 25, 50 mg/kg, respectively). Rats treated with INF39 shows a significant reduction of macroscopic damage score (4.7 at 12.5 mg/kg, 3.1 at 25 mg/kg, and 2.8 at 50 mg/kg).
Cell Research	Human THP-1 cells were exposed to INF39 (0.1?100 μM, 72 h), and then cell viability was evaluated by the MTT assay.
Animal Research	Animal Models: Male Sprague?Dawley rats. Solvent: olive oil. Dosages: 12.5,25.0,50.0 mg/kg/day,p.o.

Solubility Information

Solubility	DMSO: 10 mg/mL (44.51 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 (4.45 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	4.4508 mL	22.2539 mL	44.5077 mL
5 mM	0.8902 mL	4.4508 mL	8.9015 mL
10 mM	0.4451 mL	2.2254 mL	4.4508 mL
50 mM	0.089 mL	0.4451 mL	0.8902 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

Cocco M, et al. J Med Chem. 2017, 60(9):3656-3671.