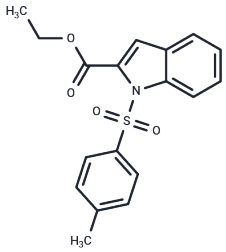
Data Sheet (Cat.No.T3587)

TargetMol

NOD-IN-1

Chemical Properties



CAS No. : 132819-92-2

Formula: C18H17NO4S

Molecular Weight: 343.4

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	NOD-IN-1 (Compound 4) is a potent mixed inhibitor of nucleotide-binding oligomerization domain (NOD)-like receptors.
Targets(IC50)	NOD-like Receptor (NLR),NOD
In vitro	NOD-IN-1, also known as compound 4, is a potent mixed inhibitor of NOD1 and NOD2, demonstrating balanced inhibitory effects on both targets within the low micromolar range. With IC50 values of 5.74 μM for NOD1 and 6.45 μM for NOD2, NOD-IN-1 is highlighted as the most effective compound in its series, showcasing significative inhibition capabilities in the lower micromolar spectrum. Comparative analysis reveals that NOD-IN-1 is seven times less effective than Noditinib-1 at inhibiting NOD1 and lacks selective inhibitory activity towards either NOD1 or NOD2, contrasting with Noditinib-1. Nonetheless, NOD-IN-1 maintains balanced dual inhibitory activities on both targets at concentrations below 10 μM[1].
Cell Research	NOD-IN-1 is dissolved in DMSO and stored, and then diluted with appropriate medium before use[1]. An MTS assay in which the proliferation rates of HEK-Blue NOD1 cells are measured in the presence of Noditinib-1 and of the synthesized potential NOD1 inhibitor NOD-IN-1 is employed to screen these compounds for potential cytotoxicity. Cells are treated for 24 h with the compound of interest at concentrations of up to 25 μM. Comparison of the resulting metabolic activities with that of the untreated control showed that all compounds are well tolerated by HEK-Blue NOD1 cells, since their residual metabolic activities do not fall below 80% at the maximum concentration tested [1].

Solubility Information

Solubility	DMSO: 55 mg/mL (160.16 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: 2 mg/mL (5.82 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	2.9121 mL	14.5603 mL	29.1206 mL
5 mM	0.5824 mL	2.9121 mL	5.8241 mL
10 mM	0.2912 mL	1.456 mL	2.9121 mL
50 mM	0.0582 mL	0.2912 mL	0.5824 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

Kecek Plesec K, et al. Identification of indole scaffold-based dual inhibitors of NOD1 and NOD2. Bioorg Med Chem. 2016 Nov 1;24(21):5221-5234.