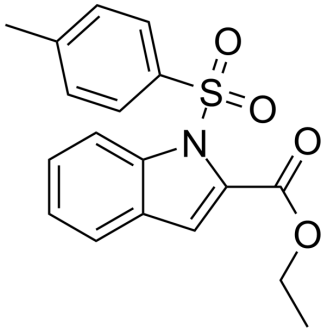
NOD-IN-1



Cat. No.:	HY-100691
CAS No.:	132819-92-2
Molecular Formula:	$C_{18}H_{17}NO_4S$
Molecular Weight:	343.4
Target:	NOD-like Receptor (NLR)
Pathway:	Immunology/Inflammation
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year

SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (291.21 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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	1.4560 mL	2.9121 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (7.28 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.28 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.28 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NOD-IN-1 is a potent mixed inhibitor of nucleotide-binding oligomerization domain (NOD)-like receptors, NOD1 and NOD2, with IC_{50} of 5.74 μM and 6.45 μM, respectively.

IC_{50} & Target

IC50: 5.74 μM (NOD1), 6.45 μM (NOD2)[1]

In Vitro

NOD-IN-1 (compound 4) is potent mixed inhibitor of NOD1 and NOD2, displaying a balanced inhibitory activity on both targets in the low micromolar range. NOD-IN-1 (IC_{50} (NOD1)=5.74 μM; IC_{50} (NOD2)=6.45 μM) is identified as the best of the

series, possessing NOD1- and NOD2-inhibitory activities in the lower micromolar range. These results show that NOD-IN-1 is 7-fold less potent than Noditinib-1 in terms of NOD1 inhibition and completely devoid of selective activity for NOD1 or NOD2 as opposed to Noditinib-1. NOD-IN-1 exhibits balanced dual activities of less than 10 μM on the two targets[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [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].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Biomed Eng. 2021 Nov 8.
- J Hazard Mater. 2021 Jan 15;402:123527.
- Front Cell Infect Microbiol. 2020 May 5;10:196.
- Cell Signal. 2022 Feb 14;93:110283.
- Mol Oral Microbiol. 2021 Mar 14.

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REFERENCES

[1]. 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.

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