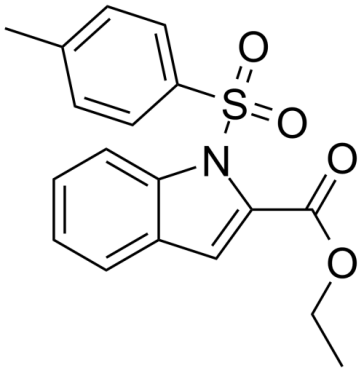
Data Sheet

Product Name:	NOD-IN-1
Cat. No.:	CS-5973
CAS No.:	132819-92-2
Molecular Formula:	$C_{18}H_{17}NO_4S$
Molecular Weight:	343.40
Target:	NOD-like Receptor (NLR)
Pathway:	Immunology/Inflammation
Solubility:	DMSO : 100 mg/mL (291.21 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

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. IC50 & 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].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: NOD-IN-1 is dissolved in DMSO and stored, and then diluted with appropriate medium before use[1]. [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].

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.

CAIndexNames:

1H-Indole-2-carboxylic acid, 1-[(4-methylphenyl)sulfonyl]-, ethyl ester

SMILES:

O=S(N1C(C(OCC)=O)=CC2=CC=CC=C21)(C3=CC=C(C)C=C3)=O

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 610-426-3128 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA