Product Data Sheet

Nodinitib-1

 $\begin{array}{lll} \textbf{Cat. No.:} & \text{HY-18639} \\ \textbf{CAS No.:} & 799264-47-4 \\ \textbf{Molecular Formula:} & C_{14}H_{13}N_3O_2S \\ \end{array}$

Molecular Weight: 287.34

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

$$0 = S = 0$$

$$N = NH_2$$

SOLVENT & SOLUBILITY

In Vitro DMSO: 20 mg/mL (69.60 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.4802 mL	17.4010 mL	34.8020 mL
	5 mM	0.6960 mL	3.4802 mL	6.9604 mL
	10 mM	0.3480 mL	1.7401 mL	3.4802 mL

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

Nodinitib-1 (ML130;CID-1088438) is a NOD1 inhibitor with an IC $_{50}$ of 0.56 $\mu\text{M}.$

In Vivo

Description

1. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (8.70 mM); Clear solution

BIOLOGICAL ACTIVITY

IC ₅₀ & Target	IC50: $0.56 \mu\text{M} (\text{NOD1})^{[1]}$
In Vitro	Nodinitib-1 selectively inhibits IL-8 production induced by NOD1 ligand. Nodinitib-1 also inhibits γ -tri-DAP-induced expression of the prototypical NF- κ B target gene I κ B α at the mRNA level. Nodinitib-1 inhibits γ -tri-DAP-dependent activation of NF- κ B (I κ B α phosphorylation and degradation) and MAPK (p38 phosphorylation) signalings, without affecting Akt survival pathway. Nodinitib-1 selectively inhibits responses of primary dendritic cells to NOD1 ligand. Nodinitib-1 reduces cell surface expression of co-stimulatory molecules CD83, CD86 and HLA-DR and also inhibits expression of IL-1 β , IL-6 and TNF α elicited by γ -tri-DAP (but not by LPS), without causing cytoxicity ^[1] . Nodinitib-1 is identified as NOD1-selective molecules from an HTS campaign involving ~290,000 compounds. Nodinitib-1 inhibits γ -tri-DAP-stimulated luciferase production in HEK 293T cells, which has endogenous NOD1 levels at submicromolar concentration as determined in a NF- κ B-linked

reporter assay^[2].

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

PROTOCOL

Cell Assay [1]

RAW264.7 cells are treated with 5 μ M of CID-1088438 or CID-44229067 alone, or also infected with S. typhimurium at multiplicity of infection (MOI) of 20 and 200 bacteria per mammalian cell. Cell viability is analyzed two hours after Salmonella infection by measuring ATP levels. Percentage viability is calculated according to the ATP levels of respective non-infected cells. Values presented are averages of two replicates (+ SEM)^[1].

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

CUSTOMER VALIDATION

- Protein Cell. 2024 Mar 4:pwae005.
- J Exp Clin Cancer Res. 2023 Sep 9;42(1):236.
- Front Immunol. 2018 Jul 2;9:1528.
- Front Pharmacol. 2022 Jul 22;13:920928.
- Cell Signal. 2022 Feb 14;93:110283.

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REFERENCES

[1]. Correa RG, et al. Discovery and characterization of 2-aminobenzimidazole derivatives as selective NOD1 inhibitors. Chem Biol. 2011 Jul 29;18(7):825-32.

[2]. Hershberger PM, et al. Synthesis and physicochemical characterization of novel phenotypic probes targeting the nuclear factor-kappa B signaling pathway. Beilstein J Org Chem. 2013 May 8;9:900-7.

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

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