

# Product data sheet



MedKoo Cat#: 532189 Name: ML130 CAS: 799264-47-4 Chemical Formula: C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S Exact Mass: 287.0728 Molecular Weight: 287.337		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

## 1. Product description:

ML130 is an inhibitor of NOD1 (nucleotide-binding oligomerization domain containing 1).

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	20.0	69.60
DMF:PBS (pH 7.2) (1:8)	0.11	0.38
DMSO	29.68	103.30
Ethanol	2.44	8.47

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.48 mL	17.40 mL	34.80 mL
5 mM	0.70 mL	3.48 mL	6.96 mL
10 mM	0.35 mL	1.74 mL	3.48 mL
50 mM	0.07 mL	0.35 mL	0.70 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

1. Lu J, Fang K, Wang S, Xiong L, Zhang C, Liu Z, Guan X, Zheng R, Wang G, Zheng J, Wang F. Anti-Inflammatory Effect of Columbianetin on Lipopolysaccharide-Stimulated Human Peripheral Blood Mononuclear Cells. *Mediators Inflamm.* 2018 Apr 5;2018:9191743. doi: 10.1155/2018/9191743. PMID: 29849500; PMCID: PMC5907401.

2. Correa RG, Khan PM, Askari N, Zhai D, Gerlic M, Brown B, Magnuson G, Spreafico R, Albani S, Sergienko E, Diaz PW, Roth GP, Reed JC. Discovery and characterization of 2-aminobenzimidazole derivatives as selective NOD1 inhibitors. *Chem Biol.* 2011 Jul 29;18(7):825-32. doi: 10.1016/j.chembiol.2011.06.009. PMID: 21802003; PMCID: PMC3152441.

### In vivo study

1. Jiang HY, Najmeh S, Martel G, MacFadden-Murphy E, Farias R, Savage P, Leone A, Roussel L, Cools-Lartigue J, Gowing S, Berube J, Giannias B, Bourdeau F, Chan CHF, Spicer JD, McClure R, Park M, Rousseau S, Ferri LE. Activation of the pattern recognition receptor NOD1 augments colon cancer metastasis. *Protein Cell.* 2020 Mar;11(3):187-201. doi: 10.1007/s13238-019-00687-5. Epub 2020 Jan 19. PMID: 31956962; PMCID: PMC7026222.

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## 7. Bioactivity

### Biological target:

Nodinitib-1 (ML130; CID-1088438) is a NOD1 inhibitor with an IC<sub>50</sub> of 0.56  $\mu$ M.

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### In vitro activity

Using a high throughput screening (HTS) assay measuring NOD1-induced NF- $\kappa$ B reporter gene activity, followed by multiple downstream counter screens that eliminated compounds impacting other NF- $\kappa$ B effectors, 2-aminobenzimidazole compounds were identified that selectively inhibit NOD1. Mechanistic studies of a prototypical compound, Nodinitib-1 (ML130; CID-1088438), suggest that these small molecules cause conformational changes of NOD1 in vitro and alter NOD1 subcellular targeting in cells.

Reference: Chem Biol. 2011 Jul 29;18(7):825-32. <https://pubmed.ncbi.nlm.nih.gov/21802003/>

### In vivo activity

The in vivo effects of NOD1 activation with C12 and co-incubation with ML130 were assessed by injecting thus treated murine MC38 colon cancer cells intrasplenically into wildtype C57BL6 mice. This study observed a significantly higher number of CRC metastatic deposits in the C12 stimulated group ( $37 \pm 7$ ) compared to DMSO control ( $3 \pm 1$ ) and ML130 co-incubated group ( $14 \pm 8$ ) ( $P = 0.0279$ ) (Fig. 3). NOD1 activation indeed augments CRC metastasis, and this effect can be attenuated by NOD1 inhibition.

Reference: Protein Cell. 2020 Mar;11(3):187-201. <https://pubmed.ncbi.nlm.nih.gov/31956962/>

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*