MD2-IN-1

Cat. No.: HY-103483

CAS No.: 111797-22-9

Molecular Formula: $C_{20}H_{22}O_6$

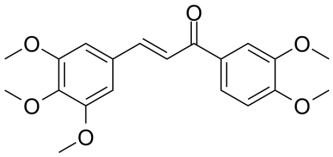
Molecular Weight: 358.39

Target: Toll-like Receptor (TLR)

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 : 50 mg/mL (139.51 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.7903 mL	13.9513 mL	27.9026 mL
5 mM	0.5581 mL	2.7903 mL	5.5805 mL
10 mM	0.2790 mL	1.3951 mL	2.7903 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: ≥ 3.25 mg/mL (9.07 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 3.25 mg/mL (9.07 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3.25 mg/mL (9.07 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MD2-IN-1 is an inhibitor of Myeloid differentiation protein 2 (MD2) with a KD of 189 μM for the recombinant human MD2 (rhMD2).

IC_{50} & Target

KD: 189 μM (rhMD2)[1]

In Vitro

Myeloid differentiation protein 2 (MD2) is a co-receptor of TLR4. Among those derivatives, MD2-IN-1 (compound 20) shows the strongest inhibitory effect on LPS-induced expression of both TNF-α and IL-6. Compare to the vehicle, LPS alone largely

	increases the amount of TLR4/MD2 complex, while pretreatment with MD2-IN-1 inhibits the increase of TLR4/MD2 complex to the vehicle level. SPR analysis shows that MD2-IN-1 exhibits recognizable binding to rhMD2 protein in a dose-dependent manner, with a KD value of 189 μM, while the KD value of xanthohumol binding to MD2 is 460 μM. Pre-treatment with different doses of MD2-IN-1 dose-dependently reduces FITC-LPS binding to MD2 in cell surface membranes, with a 65% inhibition at 10 μM in terms of mean fluorescence intensity. Pretreatment with MD2-IN-1 also dose-dependently blocks LPS-induced MAPK phosphorylation in the MPMs[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Administration of MD2-IN-1 evidently reduces the LPS-induced increase in protein concentrations in BALF. The lung wet/dry weight ratio is markedly higher in the LPS-treated group than the control group, and MD2-IN-1 treatment reduces LPS-induced pulmonary edema. LPS also causes observable lung histopathologic changes, including areas of inflammatory infiltration, hemorrhage, interstitial edema, thickening of the alveolar wall, and lung tissue destruction. These histopathological changes are ameliorated in the MD2-IN-1 treatment group[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	Mouse RAW264.7 macrophages are starved for 3 h before experimentation. Cells are incubated with or without FITC-LPS (50 μg/mL) in the presence or absence of MD2-IN-1 (0.1, 1 and 10 μM) for 30 min. After incubation, macrophages are fixed with paraformaldehyde for 10 min at 4°C and washed with PBS before being analyzed by flow cytometry[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Male Sprague Dawley (SD) rats are randomly divided into three groups, designated “control” (5 rats, only receive the vehicle of 0.9% saline), “LPS” (7 rats, receive 5 mg/kg LPS alone) and “MD2-IN-1 (20) + LPS” (6 rats, receive both MD2-IN-1 and 5 mg/kg LPS). Prior to LPS-induced Acute lung injury (ALI), the MD2-IN-1+LPS group rats are treated intragastrically with MD2-IN-1 at a dosage of 20 mg/kg/day continuously for one week. Under ether anesthesia, all the rats are exposed their trachea and challenged with intratracheal instillation of 50 μL of LPS, while the control group challenged with intratracheal instillation of 50 μL of 0.9% saline. Rats are then euthanized with ketamine after 6 h of LPS induction[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Carbohydr Polym. 2023 Apr 1;305:120533.
- Biomed Pharmacother. 2023 Aug 1;165:115227.
- J Psychiatr Res. 2023 Jun 15.

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REFERENCES

[1]. Zhang Y, et al. Discovery of new MD2 inhibitor from chalcone derivatives with anti-inflammatory effects in LPS-induced acute lung injury. Sci Rep. 2016 Apr 27;6:25130.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA