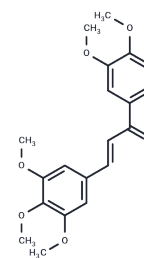


MD2-IN-1

Chemical Properties

CAS No. :	111797-22-9
Formula:	C ₂₀ H ₂₂ O ₆
Molecular Weight:	358.39
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



Biological Description

Description	MD2-IN-1 is a Myeloid differentiation protein 2 (MD2) inhibitor with a KD of 189 μ M for the recombinant human MD2 (rhMD2).
Targets(IC50)	TLR
In vitro	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 μ M in terms of mean fluorescence intensity. Pretreatment with MD2-IN-1 also dose-dependently blocks LPS-induced MAPK phosphorylation in the MPMs. Compared 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 μ M, while the KD value of xanthohumol binding to MD2 is 460 μ M.
In vivo	In the LPS-treated group, the lung wet/dry weight ratio significantly exceeds that of controls, indicating LPS-induced pulmonary edema, which MD2-IN-1 treatment effectively mitigates. Additionally, MD2-IN-1 markedly lowers the elevated protein levels in BALF caused by LPS. LPS administration results in noticeable lung histopathological alterations, such as inflammatory infiltration, hemorrhage, interstitial edema, alveolar wall thickening, and lung tissue destruction, all of which are significantly improved with MD2-IN-1 treatment.
Cell Research	Mouse RAW264.7 macrophages are starved for 3h before experimentation. Cells are incubated with or without FITC-LPS (50 μ g/mL) in the presence or absence of MD2-IN-1 (0.1, 1 and 10 μ M) for 30min. After incubation, macrophages are fixed with paraformaldehyde for 10min at 4°C and washed with PBS before being analyzed by flow cytometry.
Animal Research	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 5mg/kg LPS alone) and "MD2-IN-1 (20)+LPS" (6 rats, receive both MD2-IN-1 and 5mg/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 20mg/kg/day continuously for one week. Under ether anesthesia, all the rats are exposed their trachea and challenged with intratracheal instillation of 50 μ L of LPS, while the control group challenged with intratracheal instillation of 50 μ L of 0.9% saline. Rats are then euthanized with ketamine

A DRUG SCREENING EXPERT

Animal Research	after 6?h of LPS induction.
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Solubility Information

Solubility	DMSO: 55 mg/mL (153.46 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2.5 mg/mL (6.98 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.7903 mL	13.9513 mL	27.9026 mL
5 mM	0.5581 mL	2.7903 mL	5.5805 mL
10 mM	0.279 mL	1.3951 mL	2.7903 mL
50 mM	0.0558 mL	0.279 mL	0.5581 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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