

4-Octyl itaconate

Chemical Properties

CAS No. : 3133-16-2

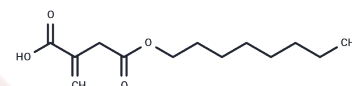
Formula: C₁₃H₂₂O₄

Molecular Weight: 242.31

Storage: Keep away from direct sunlight, Store under nitrogen,
Store at low temperature

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	4-Octyl Itaconate, a cell-permeable derivative of Itaconate, is an anti-inflammatory metabolite that activates Nrf2 via alkylation of KEAP1 and inhibits phosphorylation of STING.
Targets(IC50)	Nrf2
In vitro	<p>METHODS: Human PBMC cells were pretreated with 4-Octyl Itaconate (62.5-125 μM) for 3 h. The expression levels of target proteins were detected by Western Blot.</p> <p>RESULTS: 4-Octyl Itaconate decreased LPS-induced pro-IL-1β and HIF-1α protein levels. [1]</p> <p>METHODS: Macrophage THP1 cells were treated with 4-Octyl Itaconate (200 ng/mL) for 2 h, then stimulated with 2',3'cGAMP for 1 h. The level of p-STING was detected by Immunofluorescence.</p> <p>RESULTS: 4-Octyl Itaconate pretreatment resulted in a significant inhibition of STING phosphorylation. [2]</p>
In vivo	<p>METHODS: To test the anti-inflammatory activity in vivo, 4-Octyl Itaconate (50 mg/kg in 40% cyclodextrin in PBS) was intraperitoneally injected into mice, and 2 h later LPS (2.5 mg/kg) was intraperitoneally injected.</p> <p>RESULTS: 4-Octyl Itaconate counteracted the pro-inflammatory response to LPS in vivo. 4-Octyl Itaconate activated Nrf2, prolonged survival, decreased clinical scores and improved thermoregulation, and decreased IL-1β and TNF levels, but not IL-10, in the LPS model of sepsis. [1]</p> <p>METHODS: To investigate the role in immunosuppressive impairment in sepsis, 4-Octyl Itaconate (25-50 mg/kg) was injected intraperitoneally into a C57bl/6 mouse model of sepsis established by cecum ligation and puncture (CLP).</p> <p>RESULTS: 4-Octyl Itaconate inhibits the early release of inflammatory and oxidative stress-related factors to reduce tissue and organ damage in septic mice. [3]</p>

Solubility Information

Solubility	DMSO: 237.5 mg/mL (980.15 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 12.2 mg/mL (50.35 mM), Solution. <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>
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.1269 mL	20.6347 mL	41.2694 mL
5 mM	0.8254 mL	4.1269 mL	8.2539 mL
10 mM	0.4127 mL	2.0635 mL	4.1269 mL
50 mM	0.0825 mL	0.4127 mL	0.8254 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

Mills EL, et al. Itaconate is an anti-inflammatory metabolite that activates Nrf2 via alkylation of KEAPNature. 2018 Apr 5;556(7699):113-117.

Wang S J, Ye W, Li W Y, et al. Effects and mechanisms of Xiaochaihu Tang against liver fibrosis: An integration of network pharmacology, molecular docking and experimental validation. Journal of Ethnopharmacology. 2022: 116053.

Li W, et al. 4-octyl itaconate as a metabolite derivative inhibits inflammation via alkylation of STING. Cell Rep. 2023 Mar 28;42(3):112145.

Wang Z, Cui L, Lin Y, et al. Cancer cell-intrinsic biosynthesis of itaconate promotes tumor immunogenicity. The EMBO Journal. 2024: 1-18.

Zhang P, et al. 4-Octyl itaconate regulates immune balance by activating Nrf2 and negatively regulating PD-L1 in a mouse model of sepsis. Int J Biol Sci. 2022 Oct 24;18(16):6189-6209.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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