

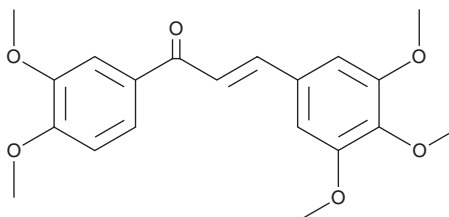
# PRODUCT INFORMATION



## MD2-IN-1

Item No. 38323

**CAS Registry No.:** 111797-22-9  
**Formal Name:** 1-(3,4-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)-2-propen-1-one  
**Synonym:** Myeloid Differentiation 2 Inhibitor 1  
**MF:** C<sub>20</sub>H<sub>22</sub>O<sub>6</sub>  
**FW:** 358.4  
**Purity:** ≥98%  
**Supplied as:** A solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

MD2-IN-1 is supplied as a solid. A stock solution may be made by dissolving the MD2-IN-1 in the solvent of choice, which should be purged with an inert gas. MD2-IN-1 is soluble in the organic solvent DMSO.

### Description

MD2-IN-1 is a chalcone derivative and an inhibitor of the interaction between myeloid differentiation 2 (MD-2) and LPS.<sup>1</sup> It inhibits the interaction between MD-2 and LPS in a cell-free assay when used at a concentration of 0.1 μM. It inhibits LPS-induced increases in the levels of TNF-α and IL-6 secreted from isolated and washed mouse peritoneal macrophages (MPMs; IC<sub>50</sub>s = 4.27 and 2.09 μM, respectively). MD2-IN-1 (5 and 20 μM) inhibits LPS-induced NF-κB DNA binding in MPMs. It inhibits the growth of HepG2 hepatocellular, A549 lung, HT-29 colon, HeLa cervical, MDA-MB-231 breast, and A2780 ovarian cancer cells (GI<sub>50</sub>s = 0.19, 0.16, 0.062, 0.019, 0.065, and 0.32 μM, respectively).<sup>2</sup> MD2-IN-1 (10 mg/kg) reduces tumor volume and weight in a HeLa mouse xenograft model. *In vivo*, MD2-IN-1 (20 mg/kg per day) prevents LPS-induced increases in bronchoalveolar lavage fluid (BALF) total protein levels and CD68<sup>+</sup> macrophage and neutrophil infiltration in a mouse model of LPS-induced acute lung injury.<sup>1</sup> It also reduces myeloperoxidase (MPO) activity in isolated neutrophils in the same model.

### References

1. Zhang, Y., Wu, J., Ying, S., *et al.* Discovery of new MD2 inhibitor from chalcone derivatives with anti-inflammatory effects in LPS-induced acute lung injury. *Sci. Rep.* **6**, 25130 (2016).
2. Zhang, Y.-L., Li, B.-Y., Yang, R., *et al.* A class of novel tubulin polymerization inhibitors exert effective anti-tumor activity via mitotic catastrophe. *Eur. J. Med. Chem.* **163**, 896-910 (2019).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 11/14/2023

#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

**PHONE:** [800] 364-9897  
[734] 971-3335

**FAX:** [734] 971-3640

CUSTSERV@CAYMANCHEM.COM  
[WWW.CAYMANCHEM.COM](http://WWW.CAYMANCHEM.COM)