

PRODUCT INFORMATION

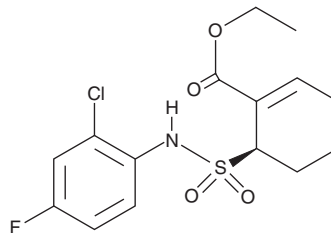


TAK-242

Item No. 13871

CAS Registry No.: 243984-11-4
Formal Name: 6R-[[[(2-chloro-4-fluorophenyl)amino]sulfonyl]-1-cyclohexene-1-carboxylic acid, ethyl ester

Synonym: Resatorvid
MF: C₁₅H₁₇NO₄ClFS
FW: 361.8
Purity: ≥98%
Supplied as: A crystalline 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

TAK-242 is supplied as a crystalline solid. A stock solution may be made by dissolving the TAK-242 in the solvent of choice, which should be purged with an inert gas. TAK-242 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of TAK-242 in ethanol is approximately 20 mg/ml and approximately 10 mg/ml in DMSO and DMF.

Description

TAK-242 is an antagonist of toll-like receptor 4 (TLR4) with an IC₅₀ value of 0.68 μM in a secreted alkaline phosphatase (SEAP) assay.¹ It selectively binds to TLR4 over TLR1-3 and TLR5-10 when used at a concentration of 100 nM.² TAK-242 (1 μM) prevents the interaction of TLR4 with its adaptor proteins TIRAP or TRAM in HEK293 cells expressing the human receptors.² It inhibits IFN-γ- and LPS-induced production of nitric oxide (NO), TNF-α, IL-6, and IL-1β in isolated mouse peritoneal macrophages (IC₅₀s = 5.7-11 nM), as well as inhibits LPS-induced NETosis in isolated human neutrophils when used at concentrations ranging from 5 to 20 μM.^{3,4} TAK-242 (0.3, 1, and 3 mg/kg) improves survival in a mouse model of septic shock induced by LPS.⁵

References

- Huang, J., Zhou, Z., Zhou, M., *et al.* Development of benzoxazole deoxybenzoin oxime and acyloxylamine derivatives targeting innate immune sensors and xanthine oxidase for treatment of gout. *Bioorg. Med. Chem.* **26(8)**, 1653-1664 (2018).
- Matsunaga, N., Tsuchimori, N., Matsumoto, T., *et al.* TAK-242 (resatorvid), a small-molecule inhibitor of Toll-like receptor (TLR) 4 signaling, binds selectively to TLR4 and interferes with interactions between TLR4 and its adaptor molecules. *Mol. Pharmacol.* **79(1)**, 34-41 (2011).
- li, M., Matsunaga, N., Hazeki, K., *et al.* A novel cyclohexene derivative, ethyl (6R)-6-[N-(2-Chloro-4-fluorophenyl)sulfamoyl]cyclohex-1-ene-1-carboxylate (TAK-242), selectively inhibits toll-like receptor 4-mediated cytokine production through suppression of intracellular signaling. *Mol. Pharmacol.* **69(4)**, 1288-1295 (2006).
- Khan, M.A., Farahvash, A., Douda, D.N., *et al.* JNK activation turns on LPS- and gram-negative bacteria-induced NADPH oxidase-dependent suicidal NETosis. *Sci. Rep.* **7(1)**, 3409 (2017).
- Yamada, M., Ichikawa, T., li, M., *et al.* Discovery of novel and potent small-molecule inhibitors of NO and cytokine production as antisepsis agents: Synthesis and biological activity of alkyl 6-(N-substituted sulfamoyl)cyclohex-1-ene-1-carboxylate. *J. Med. Chem.* **48(23)**, 7457-7467 (2005).

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.

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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