

Product Name: TAK 242

Catalog No.: 6587

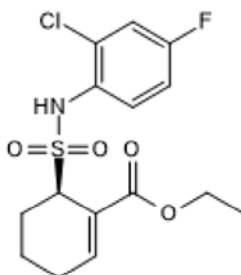
Batch No.: 2

CAS Number: 243984-11-4

IUPAC Name: (R)-Ethyl 6-(N-(2-chloro-4-fluorophenyl)sulfamoyl)cyclohex-1-enecarboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₇ClFNO₄S
Batch Molecular Weight: 361.82
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +110.7 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	49.79	4.74	3.87
Found	49.86	4.73	3.98

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Toll-like receptor 4 (TLR4) signaling inhibitor. Binds to intracellular domain of TLR4. Inhibits LPS-induced cytokine production in vitro (IC₅₀ values are 1.3, 1.3 and 3.2 nM for IL-6, TNF α and NO production). Reduces lesion volume in a mouse model of cerebral cavernous malformations (CCMs). Also attenuates increased cytokine levels in a mouse sepsis model, when given in combination with ceftazidime. Cell permeable.

Physical and Chemical Properties:

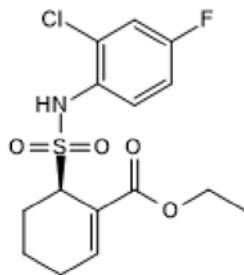
Batch Molecular Formula: C₁₅H₁₇ClFNO₄S

Batch Molecular Weight: 361.82

Physical Appearance: White solid

Minimum Purity: \geq 98%

Batch Molecular Structure:



References:

Tang et al (2017) Endothelial TLR4 and the microbiome drive cerebral cavernous malformations. *Nature* **545** 305. PMID: 28489816.

Takashima et al (2009) Analysis of binding site for the novel small-molecule TLR4 signal transduction inhibitor TAK-242 and its therapeutic effect on mouse sepsis model. *Br.J.Pharmacol.* **157** 1250. PMID: 19563534 .

li et al (2006) 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 signal *Mol.Pharmacol.* **69** 1288. PMID: 16373689.

Yamada et al (2005) 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** 7457. PMID: 16279805.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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