Print Date: Dec 11th 2018

# Certificate of Analysis

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**Product Name:** **TAK 242** **Catalog No.: 6587** **Batch No.: 1**

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:** $C_{15}H_{17}ClFNO_4S$

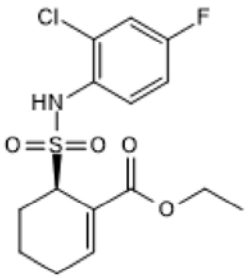
**Batch Molecular Weight:** 361.82

**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

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** $[\alpha]_D$ = +115.8 (Concentration = 1, Solvent = Methanol)

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 49.79 | 4.74 | 3.87 |
| Found | 49.84 | 4.68 | 3.88 |



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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 ($IC_{50}$ values are 1.3, 1.3 and 3.2 nM for IL-6, TNFα 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:**

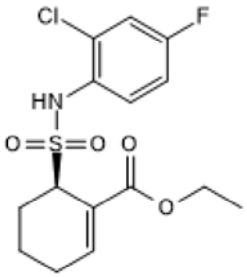
Batch Molecular Formula: $C_{15}H_{17}ClFNO_4S$

Batch Molecular Weight: 361.82

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**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.

**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 .

**Ii** *et al* (2006) A novel cyclohexene derivative, ethyl (6*R*)-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*** 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.