

# **Certificate of Analysis**

Print Date: Jul 19th 2018

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Product Name: CY 09 Catalog No.: 6436 Batch No.: 1

CAS Number: 1073612-91-5

IUPAC Name: 4-[[4-Oxo-2-thioxo-3-[[3-(trifluoromethyl)phenyl]methyl]-5-thiazolidinylidene]methyl]benzoic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>12</sub>F<sub>3</sub>NO<sub>3</sub>S<sub>2</sub>

**Batch Molecular Weight:** 423.43 **Physical Appearance:** Yellow solid

**Solubility:** DMSO to 20 mM with gentle warming

Storage: Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 98.7% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.89 2.86 3.31 Found 53.89 2.88 3.06

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## **Product Information**

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#### **Description:**

NLRP3 inhibitor ( $K_d$  = 500 nM); directly binds to ATP-binding motif of NLRP3 NACHT domain. Blocks NLRP3 inflammasome assembly and activation. Displays therapeutic effects on mouse models of cryopyrin-associated autoinflammatory syndrome (CAPS) and type 2 diabetes. Exhibits no activity for hERG (10  $\mu$ M).

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>19</sub>H<sub>12</sub>F<sub>3</sub>NO<sub>3</sub>S<sub>2</sub>

Batch Molecular Weight: 423.43 Physical Appearance: Yellow solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

#### Storage: Store at +4°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 20 mM with gentle warming

## 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:

**Jiang** et al (2017) Identification of a selective and direct NLRP3 inhibitor to treat inflammatory disorders. J.Exp.Med. **214** 3219. PMID: 29021150.