

**Certificate of Analysis** 

Print Date: Jan 13<sup>th</sup> 2017

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Product Name: CCF 642 Catalog No.: 6063 Batch No.: 1

CAS Number: 346640-08-2

**Batch Molecular Structure:** 

IUPAC Name: 3-(4-Methoxyphenyl)-5-[(5-nitro-2-thienyl)methylene]-2-thioxo-4-thiazolidinone

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{15}H_{10}N_2O_4S_3$ 

Batch Molecular Weight:378.45Physical Appearance:Brown solidSolubility:DMSO to 20 mMStorage:Store at -20°C

O<sub>2</sub>N O

2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.61 2.66 7.4 Found 47.36 2.75 7.36



# **Product Information**

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### **Description:**

Protein disulfide isomerase (PDI) inhibitor. Induces acute ER stress and apoptosis in multiple myeloma cells in vitro (submicromolar activity). Prolongs survival of C57BL/KaLwRij mice engrafted with 5TGM1-luc myeloma. Also a bone marrow-sparing compound.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>S<sub>3</sub> Batch Molecular Weight: 378.45 Physical Appearance: Brown 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 20 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:

Vatolin et al (2016) Novel protein disulfide isomerase inhibitor with anticancer activity in multiple myeloma. Cancer Res. 76 3340. PMID: 27197150.