TOCRIS
a bio-techne brand

Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **AI-3** **Catalog No.: 5145** **Batch No.: 1**

CAS Number: 882288-28-0

IUPAC Name: 1-Chloro-6,7-dihydro-6,6-dimethyl-3-(methylsulfonyl)-benzo[*c*]thiophen-4(5*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_{13}ClO_3S_2$

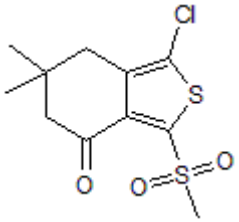
Batch Molecular Weight: 292.8

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	45.12	4.48	
Found	44.93	4.38	

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Description:

Antioxidant response element (ARE) activator; disrupts Nrf2/Keap1 and Keap1/Cul3 interactions and stabilizes Nrf2. Activates ARE in an Nrf2 and PI 3-kinase dependent manner. Induces cytoprotective gene expression in vitro and in vivo.

Physical and Chemical Properties:

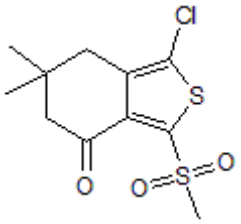
Batch Molecular Formula: $C_{11}H_{13}ClO_3S_2$

Batch Molecular Weight: 292.8

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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:

Wang *et al* (2013) In vitro and in vivo characterization of a tunable dual-reactivity probe of the Nrf2-ARE pathway. ACS Chem.Biol. ***8*** 1764. PMID: 23773140.