# **Certificate of Analysis**

# www.tocris.com

Catalog No.: 7353

## Product Name: MSA 2

CAS Number: 129425-81-6 IUPAC Name: 4-(5,6-Dimethoxybenzo[b]thiophen-2-yl)-4-oxobutanoic acid

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: **Batch Molecular Weight:** Physical Appearance: Solubility: Storage: **Batch Molecular Structure:**   $C_{14}H_{14}O_5S$ 294.32 Off White solid DMSO to 100 mM Store at -20°C

-OH

## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis:

Shows 99.5% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 57.13 4.79 Found 56.88 4.78

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

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Print Date: Dec 17th 2020

Batch No.: 1

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# **Product Information**

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Print Date: Dec 17th 2020

## Product Name: MSA 2

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Batch No.: 1

CAS Number: 129425-81-6 IUPAC Name: 4-(5,6-Dimethoxybenzo[*b*]thiophen-2-yl)-4-oxobutanoic acid

### **Description:**

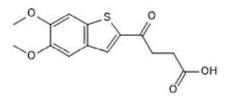
Non-nucleotide STING agonist (EC<sub>50</sub> values are 8.3 and 24  $\mu$ M for human STING isoforms WT and HAQ, respectively). Exhibits antitumor activity and stimulates interferon- $\beta$  secretion in tumors. Induces tumor regression with durable antitumor immunity, and synergizes with anti-PD-1 in syngeneic mouse tumor models. Orally bioavailable.

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

Batch Molecular Formula: C<sub>14</sub>H<sub>14</sub>O<sub>5</sub>S Batch Molecular Weight: 294.32 Physical Appearance: Off White solid

Minimum Purity: ≥98%

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



#### **Storage:** Store at -20°C

Solubility & Usage Info: DMSO 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:**

Pan et al (2020) An orally available non-nucleotide STING agonist with antitumor activity. Science 369 eaba6098. PMID: 32820094.

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