

**Product Name:** 

# **Certificate of Analysis**

Print Date: May 20th 2022

www.tocris.com

ACET Catalog No.: 2728 Batch No.: 6

CAS Number: 936095-50-0

**Batch Molecular Structure:** 

IUPAC Name: (S)-1-(2-Amino-2-carboxyethyl)-3-(2-carboxy-5-phenylthiophene-3-yl-methyl)-5-methylpyrimidine-2,4-dione

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{20}H_{19}N_3O_6S.^3/4H_2O$ 

Batch Molecular Weight: 442.96

Physical Appearance: Off White solid

**Solubility:** DMSO to 20 mM 3eq. NaOH to 10 mM

**Storage:** Store at RT

#### 2. ANALYTICAL DATA

**HPLC:** Shows 98.9% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.23 4.66 9.49 Found 54.17 4.32 9.48

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



# **Product Information**

Print Date: May 20th 2022

www.tocris.com

Product Name: ACET Catalog No.: 2728 Batch No.: 6

CAS Number: 936095-50-0

IUPAC Name: (S)-1-(2-Amino-2-carboxyethyl)-3-(2-carboxy-5-phenylthiophene-3-yl-methyl)-5-methylpyrimidine-2,4-dione

#### **Description:**

ACET is a potent and selective GluK1 (formerly GluR5) containing kainate receptor antagonist (IC $_{50}$  = 7 nM) that displays selectivity over GluK2 (formerly GluR6) containing kainate, NMDA, AMPA and group I mGlu receptors. Reversibly blocks induction of NMDA receptor-independent long term potentiation (LTP) in vitro at nanomolar concentrations. Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>19</sub>N<sub>3</sub>O<sub>6</sub>S.<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 442.96 Physical Appearance: Off White solid

**Minimum Purity**: ≥98%

# **Batch Molecular Structure:**

$$H_2N$$
 $CO_2H$ 
 $CO_2H$ 

Storage: Store at RT

## Solubility & Usage Info:

DMSO to 20 mM 3eq. NaOH to 10 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:

**Dargan** et al (2009) ACET is a highly potent and specific kainate receptor antagonist: Characterisation and effects on hippocampal mossy fibre function. Neuropharmacology **56** 121. PMID: 18789344.

**Dolman** *et al* (2007) Synthesis and pharmacological characterisation of N3-substituted willardiine derivatives: role of the substituent at the 5-position of the uracil ring in the development of highly potent and selective GLUK5 kainate receptor antagonis J.Med.Chem. *50* 1558. PMID: 17348638.

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