# TOCRIS a biotechne brand

#### Print Date: Sep 19th 2018

# **Certificate of Analysis**

## www.tocris.com

### Product Name: AR-C155858

# Catalog No.: 4960 Batch No.: 3

CAS Number: IUPAC Name:

6-[(3,5-Dimethyl-1*H*-pyrazol-4-yl)methyl]-5-[[(4*S*)-4-hydroxy-2-isoxazolidinyl]carbonyl]-3-methyl-1-(2-methylpropyl) thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione

# 1. PHYSICAL AND CHEMICAL PROPERTIES

496791-37-8

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure:  $C_{21}H_{27}N_5O_5S.^{1}H_2O$ 470.54 White solid DMSO to 100 mM Store at -20°C



## 2. ANALYTICAL DATA

TLC: HPLC: Chiral HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: R<sub>f</sub> = 0.4 (Dichloromethane:Methanol [85:15]) Shows 99.6% purity Shows 99% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 53.6 6 14.88

5.99

14.76

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

53.57

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Found

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#### **Description:**

Inhibitor of the monocarboxylate transporters (MCTs) MCT1 and MCT2 ( $K_i$  values are 2.3 and <10 nM respectively). Exhibits no activity at MCT4. Blocks proliferation of Raji lymphoma cells in vitro. Inhibits glycolysis and glutathione synthesis in cancer cells.

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

Batch Molecular Formula:  $C_{21}H_{27}N_5O_5S.^{1/2}H_2O$ Batch Molecular Weight: 470.54 Physical Appearance: 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.

#### Licensing Information:

Sold for research purposes under agreement from AstraZeneca UK Limited

#### **References:**

**Doherty** *et al* (2014) Blocking lactate export by inhibiting the Myc target MCT1 Disables glycolysis and glutathione synthesis. Cancer Res. **74** 908. PMID: 24285728.

**Ovens** *et al* (2010) The inhibition of monocarboxylate transporter 2 (MCT2) by AR-C155858 is modulated by the associated ancillary protein. Biochem.J. **431** 217. PMID: 20695846.

**Ovens** *et al* (2010) AR-C155858 is a potent inhibitor of monocarboxylate transporters MCT1 and MCT2 that binds to an intracellular site involving transmembrane helices 7-10. Biochem.J. **425** 523. PMID: 19929853.

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