

# **Certificate of Analysis**

Print Date: May 29th 2019

www.tocris.com

**PU 23 Product Name:** Catalog No.: 6885 Batch No.: 1

CAS Number: 817635-93-1

**IUPAC Name:** N-[[[4-[[(Phenylmethyl)amino]sulfonyl]phenyl]amino]thioxomethyl]benzamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{21}H_{19}N_3O_3S_2$ **Batch Molecular Formula:** 

**Batch Molecular Weight:** 425.52

**Physical Appearance:** Off White solid DMSO to 50 mM Solubility: Store at -20°C Storage:

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

HPLC: Shows 98% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 59.27 4.5 9.87 Found 59.34 4.49 9.88

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

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## **Product Information**

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## **Description:**

Multidrug resistance protein (MRP) 4 inhibitor. Sensitizes MRP4-overexpressing cells to the anticancer agent 6-Mercaptopurine (Cat. No. 4103; 6-MP) (IC $_{50}$  values are 14.11 and 6.06  $\mu$ M in the absence and presence of compound, respectively). Increases accumulation of 6-MP in MRP4-overexpressing cells.

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

Batch Molecular Formula: C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>

Batch Molecular Weight: 425.52 Physical Appearance: Off White solid

Minimum Purity: >98%

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

Storage: Store at -20°C

### Solubility & Usage Info:

DMSO 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:

**Chen** *et al* (2018) Discovery of novel multidrug resistance protein 4 (MRP4) inhibitors as active agents reducing resistance to anticancer drug 6-Mercaptopurine (6-MP) by structure and ligand-based virtual screening. PLoS One *13* e0205175. PMID: 30321196.

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