

**Product Name:** PKUMDL WQ 2201

**Catalog No.:** 6581

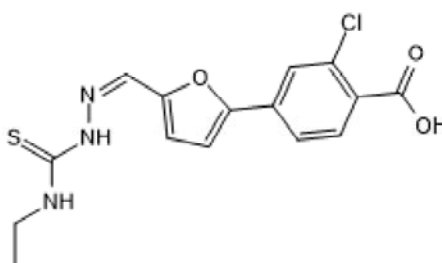
**Batch No.:** 1

CAS Number: 592474-91-4

IUPAC Name: 2-Chloro-4-[5-[[2-[(ethylamino)thioxomethyl]hydrazinylidene]methyl]-2-furanyl]benzoic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>15</sub>H<sub>14</sub>ClN<sub>3</sub>O<sub>3</sub>S  
**Batch Molecular Weight:** 351.81  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**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	51.21	4.01	11.94
Found	51.22	3.94	11.91

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

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**Description:**

Negative allosteric modulator of phosphoglycerate dehydrogenase (PHGDH) ( $IC_{50} = 35.7 \mu M$ ). Displays dose-dependent suppression of cell viability in a range of cancer cell lines. Inhibits tumor growth in a xenograft mouse model.

**Physical and Chemical Properties:**

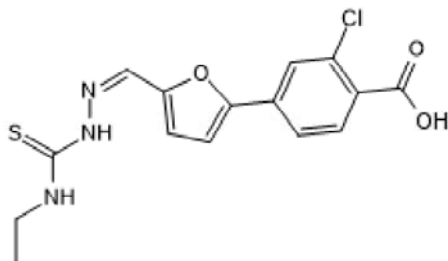
Batch Molecular Formula:  $C_{15}H_{14}ClN_3O_3S$

Batch Molecular Weight: 351.81

Physical Appearance: Yellow 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:**

**Wang et al** (2017) Rational design of selective allosteric inhibitors of PHGDH and serine synthesis with anti-tumor activity. *Cell Chem.Biol.* **24** 55. PMID: 28042046 .

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