

Certificate of Analysis

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Product Name: PKUMDL WQ 2101

Catalog No.: 6580

Batch No.: 1

CAS Number: 304481-72-9

IUPAC Name: C₁₄H₁₁N₃O₆

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₁N₃O₆·¼H₂O

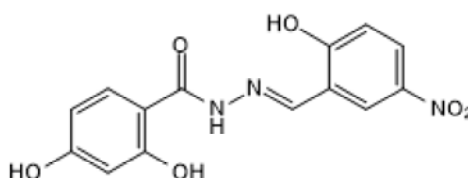
Batch Molecular Weight: 321.75

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.26	3.6	13.06
Found	52.32	3.52	13.18

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

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Batch No.: 1

CAS Number: 304481-72-9

IUPAC Name: C₁₄H₁₁N₃O₆

Description:

Negative allosteric modulator of phosphoglycerate dehydrogenase (PHGDH) (IC₅₀ = 34.8 μM). Exhibits antitumor activity in vitro in breast cancer cells lines overexpressing PHGDH (EC₅₀ values are 7.7 and 10.8 μM in MDA-MB-468 and HCC-70 cells, respectively). Inhibits growth of MDA-MB-468 xenografts in mice.

Physical and Chemical Properties:

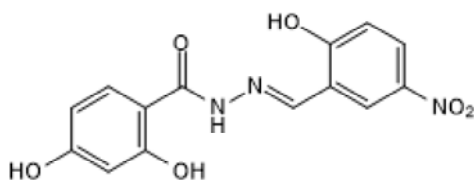
Batch Molecular Formula: C₁₄H₁₁N₃O₆·¼H₂O

Batch Molecular Weight: 321.75

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



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.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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.

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