

Certificate of Analysis

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Product Name: YZ9

Catalog No.: 5048

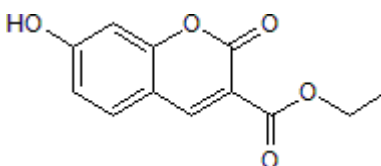
Batch No.: 1

CAS Number: 6093-71-6

IUPAC Name: Ethyl 7-hydroxy-2-oxo-2H-1-benzopyran-3-carboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₂H₁₀O₅·H₂O
Batch Molecular Weight: 252.22
Physical Appearance: Beige solid
Solubility: DMSO to 50 mM
ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.15	4.8	
Found	57.18	4.81	

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

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IUPAC Name: Ethyl 7-hydroxy-2-oxo-2H-1-benzopyran-3-carboxylate

Description:

PFKFB3 (6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase) inhibitor ($IC_{50} = 0.183 \mu M$). Also competitively inhibits F-6-P ($K_i = 0.094 \mu M$). Inhibits cell growth ($GI_{50} = 2.7 \mu M$) in a XTT-based in vitro toxicology assay.

Physical and Chemical Properties:

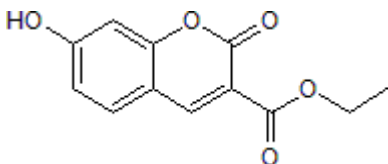
Batch Molecular Formula: $C_{12}H_{10}O_5 \cdot H_2O$

Batch Molecular Weight: 252.22

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM
ethanol to 20 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:

Seo *et al* (2011) Structure-based development of small molecule PFKFB3 inhibitors: a framework for potential cancer therapeutic agents targeting the Warburg effect. *PLoS One* **6** e24179. PMID: 21957443.

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