

Product Name: CFTR_{inh} 172

Catalog No.: 3430

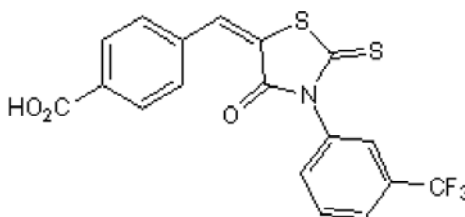
Batch No.: 3

CAS Number: 307510-92-5

IUPAC Name: 4-[[4-Oxo-2-thioxo-3-[3-trifluoromethyl)phenyl]-5-thiazolidinylidene]methyl]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₀F₃NO₃S₂
Batch Molecular Weight: 409.4
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.81	2.46	3.42
Found	53.01	2.34	3.52

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

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Description:

Voltage-independent, selective CFTR chloride channel blocker ($K_i = 300$ nM) that alters channel gating. Blocks intestinal fluid secretion induced by cholera toxin and Escherichia coli and suppresses cyst growth in animal models of polycystic kidney disease. Orally active. Inhibits mitochondrial respiration and increases reactive oxygen species (ROS) production independently of CFTR in several cell lines.

Physical and Chemical Properties:

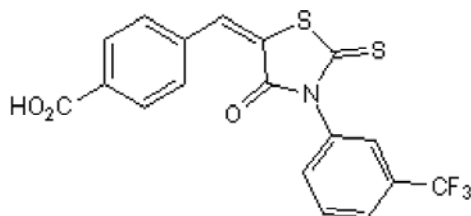
Batch Molecular Formula: C₁₈H₁₀F₃NO₃S₂

Batch Molecular Weight: 409.4

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Kelly et al (2010) Cystic fibrosis transmembrane regulator inhibitors CFTR_{inh}-172 and GlyH-101 target mitochondrial functions, independently of chloride channel inhibition. *J.Pharmacol.Exp.Ther.* **333** 60.

Rafferty et al (2009) Rescue of functional F508del cystic fibrosis transmembrane conductance regulator by vasoactive intestinal peptide in the human nasal epithelial cell line JME/CF15. *J.Pharmacol.Exp.Ther.* **331** 2. PMID: 19584307.

Yang et al (2008) Small-molecule CFTR inhibitors slow cyst growth in polycystic kidney disease. *J.Am.Soc.Nephrol.* **19** 1300. PMID: 18385427.

Taddei et al (2004) Altered channel gating mechanism for CFTR inhibition by a high-affinity thiazolidinone blocker. *FEBS Lett.* **558** 52. PMID: 14759515.

Ma et al (2002) Thiazolidinone CFTR inhibitor identified by high-throughput screening blocks cholera toxin-induced intestinal fluid secretion. *J.Clin.Invest.* **110** 1651. PMID: 12464670.

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