

Product Name: CCT 018159

Catalog No.: 2435

Batch No.: 4

CAS Number: 171009-07-7

IUPAC Name: 4-[4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-5-methyl-1H-pyrazol-3-yl]-6-ethyl-1,3-benzenediol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₀N₂O₄·1½H₂O

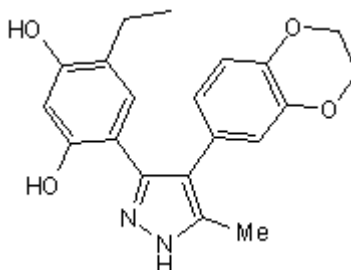
Batch Molecular Weight: 374.91

Physical Appearance: white solid

Solubility: water to 5 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ether:Petroleum ether [7:3])

HPLC: Shows >99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.07	6.05	7.47
Found	64.31	6.12	7.44

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

Product Name: CCT 018159

Catalog No.: 2435

Batch No.: 4

CAS Number: 171009-07-7

IUPAC Name: 4-[4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-5-methyl-1H-pyrazol-3-yl]-6-ethyl-1,3-benzenediol

Description:

Novel inhibitor of heat shock protein 90 (Hsp90) ATPase activity ($IC_{50} = 5.7 \mu\text{M}$) that displays selectivity over human Hsp72 and topoisomerase II. Inhibits proliferation of HCT116 human colon tumor cells and produces upregulation of Hsp70 and downregulation of c-Raf and cdk4. More soluble than 17-AAG (Cat. No. 1515) and is independent of NQO1/DT-diaphorase and P-glycoprotein expression.

Physical and Chemical Properties:

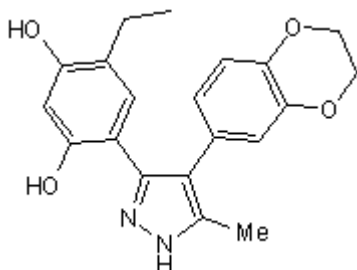
Batch Molecular Formula: $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_4 \cdot 1\frac{1}{4}\text{H}_2\text{O}$

Batch Molecular Weight: 374.91

Physical Appearance: white solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Cheung et al (2005) The identification, synthesis, protein crystal structure and in vitro biochemical evaluation of a new 3,4-diarylpyrazole class of Hsp90 inhibitors. *Bioorg.Med.Chem.Lett.* **15** 3338. PMID: 15955698.

Dymock et al (2005) Novel, potent small-molecule inhibitors of the molecular chaperone Hsp90 discovered through structure-based design. *J.Med.Chem.* **48** 4212. PMID: 15974572.

Sharp et al (2007) *In vitro* biological characterization of a novel, synthetic diaryl pyrazole resorcinol class of heat shock protein 90 inhibitors. *Cancer Res.* **67** 2206. PMID: 17332351.

Storage: Store at +4°C

Solubility & Usage Info:

water to 5 mM
DMSO to 100 mM
ethanol 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.

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