

**Product Name:** CCT 018159

**Catalog No.:** 2435

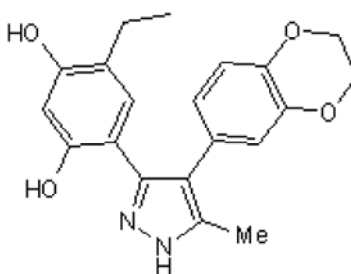
**Batch No.:** 5

CAS Number: 171009-07-7

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

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>  
**Batch Molecular Weight:** 352.39  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	68.17	5.72	7.95
Found	68.15	5.77	7.9

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

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**Description:**

CCT 018159 is a novel inhibitor of heat shock protein 90 (Hsp90) ATPase activity (IC<sub>50</sub> = 5.7 μM) 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:**

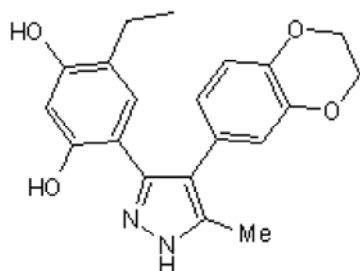
Batch Molecular Formula: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>

Batch Molecular Weight: 352.39

Physical Appearance: White 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:**

**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.

**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.

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