

## Certificate of Analysis

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**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:**  $C_{20}H_{20}N_2O_4 \cdot 1\frac{1}{4}H_2O$

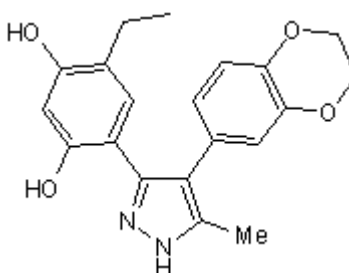
**Batch Molecular Weight:** 374.91

**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

**<sup>1</sup>H 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

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**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:**

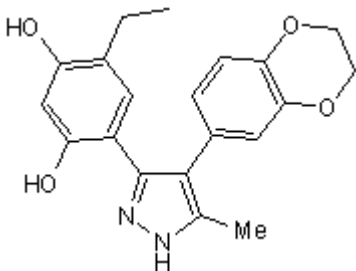
Batch Molecular Formula:  $C_{20}H_{20}N_2O_4 \cdot 1 \frac{1}{4} H_2O$

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.

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