

**Product Name:** PMX 464

**Catalog No.:** 4996

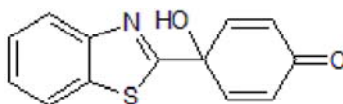
**Batch No.:** 2

CAS Number: 485842-97-5

IUPAC Name: 4-(2-Benzothiazolyl)-4-hydroxy-2,5-cyclohexadien-1-one

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>13</sub>H<sub>9</sub>NO<sub>2</sub>S.H<sub>2</sub>O  
**Batch Molecular Weight:** 261.3  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.76	4.24	5.36
Found	60	4.59	5.43

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

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**Description:**

Putative inhibitor of the thioredoxin-thioredoxin reductase (Trx-TrxR) system. Shown to inhibit Trx and induce a G<sub>1</sub>/S block in HT29 cells; inhibits cell proliferation in various colorectal cancer cell lines and MCF7 cells. Also elicits an anti-inflammatory response in A549 cells.

**Physical and Chemical Properties:**

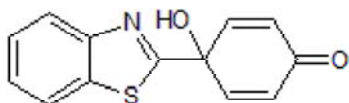
Batch Molecular Formula: C<sub>13</sub>H<sub>9</sub>NO<sub>2</sub>S.H<sub>2</sub>O

Batch Molecular Weight: 261.3

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

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.

**References:**

**Callister et al** (2008) PMX464, a thiol-reactive quinol and putative thioredoxin inhibitor, inhibits NF-κB-dependent proinflammatory activation of alveolar epithelial cells. *Br.J.Pharmacol.* **155** 661. PMID: 18587424.

**Mukherjee et al** (2007) A cellular and molecular investigation of the action of PMX464, a putative thioredoxin inhibitor, in normal and colorectal cancer cell lines. *Br.J.Pharmacol.* **151** 1167. PMID: 17572693.

**Mukherjee et al** (2005) Cytotoxic and antiangiogenic activity of AW464 (NSC 706704), a novel thioredoxin inhibitor: an *in vitro* study. *Br.J.Cancer* **92** 350. PMID: 15655539.

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