

**Product Name:** PYR 41

**Catalog No.:** 2978

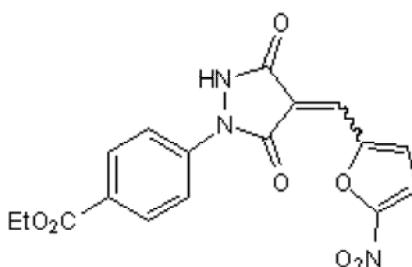
**Batch No.:** 3

CAS Number: 418805-02-4

IUPAC Name: 4-[4-[(5-Nitro-2-furanyl)methylene]-3,5-dioxo-1-pyrazolidinyl]benzoic acid ethyl ester

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>O<sub>7</sub>  
**Batch Molecular Weight:** 371.3  
**Physical Appearance:** Brown solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.99	3.53	11.32
Found	55	3.51	11.25

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

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**Description:**

Cell-permeable, irreversible ubiquitin-activating enzyme (E1) inhibitor ( $IC_{50} < 10 \mu M$ ). Blocks ubiquitination and prevents ubiquitin-mediated proteasomal degradation. Inhibits NF- $\kappa B$  activation, blocks degradation of p53, increases p21 levels and induces apoptosis in vitro. Also causes an increase in sumoylation of proteins.

**Physical and Chemical Properties:**

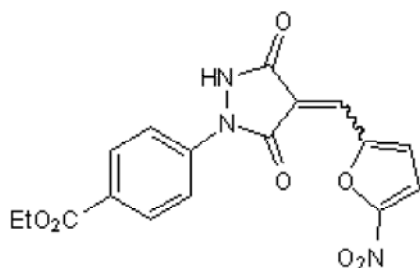
Batch Molecular Formula:  $C_{17}H_{13}N_3O_7$

Batch Molecular Weight: 371.3

Physical Appearance: Brown solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}C$

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**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  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Brahmi et al** (2010) Homology modelling of human E1 ubiquitin activating enzyme. *Lett. Drug Des. Discov.* **7** 57. PMID: 20396627.

**Mi et al** (2009) Cancer preventative isothiocyanates induce selective degradation of cellular  $\alpha$ - and  $\beta$ -tubulins by proteasomes. *J. Biol. Chem.* **284** 17039. PMID: 19339240.

**Yang et al** (2007) Inhibitors of ubiquitin-activating enzyme (E1), a new class of potential cancer therapeutics. *Cancer Res.* **67** 9472. PMID: 17909057.

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