

**Product Name:** PD 0332991 isethionate

**Catalog No.:** 4786

**Batch No.:** 4

CAS Number: 827022-33-3

IUPAC Name: 6-acetyl-8-cyclopentyl-5-methyl-2-[[5-(1-piperazinyl)-2-pyridinyl]amino]pyrido[2,3-*d*]pyrimidin-7(8*H*)-one isethionate salt

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>·C<sub>2</sub>H<sub>6</sub>O<sub>4</sub>S·1½H<sub>2</sub>O

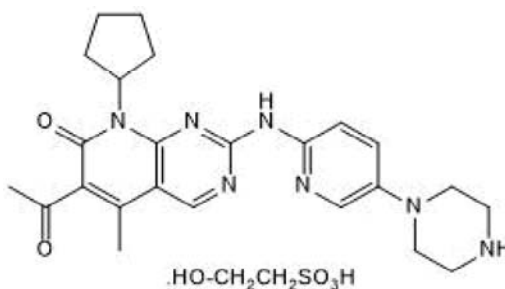
**Batch Molecular Weight:** 600.68

**Physical Appearance:** Yellow solid

**Solubility:** water to 100 mM  
DMSO to 10 mM

**Storage:** Desiccate at RT

**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	51.99	6.38	16.32
Found	51.86	6.32	16.17

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**Description:**

PD 0332991 isethionate is a potent cyclin-dependent kinase 4 (cdk4) and cdk6 inhibitor (IC<sub>50</sub> values are 11 nM and 15 nM respectively). Also displays activity at cdk2, cdk5 and cdk9 (IC<sub>50</sub> values reported to be 1.6, 1.8 and 0.42-1.1 μM, respectively). Induces G1 cell cycle arrest and senescence in retinoblastoma protein (Rb)-proficient cell lines; blocks growth of intracranial glioblastoma multiforme xenografts in mice. Brain penetrant.

**Physical and Chemical Properties:**

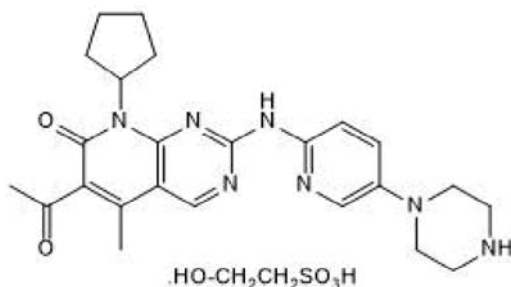
Batch Molecular Formula: C<sub>24</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>.C<sub>2</sub>H<sub>6</sub>O<sub>4</sub>S.1½H<sub>2</sub>O

Batch Molecular Weight: 600.68

Physical Appearance: Yellow solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**References:**

Jorda *et al* (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? *J.Med.Chem.* **61** 9105. PMID: 30234987.

Michaud *et al* (2010) Pharmacologic inhibition of cyclin-dependent kinases 4 and 6 arrests the growth of glioblastoma multiforme intracranial xenografts. *Cancer Res.* **70** 3228. PMID: 20354191.

Toogood *et al* (2005) Discovery of a potent and selective inhibitor of cyclin-dependent kinase 4/6. *J.Med.Chem.* **48** 2388. PMID: 15801831.

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 100 mM

DMSO to 10 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.

**Licensing Information:**

Sold for research purposes under agreement from Pfizer Inc.

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