

Product Name: PD 0332991 isethionate

Catalog No.: 4786

Batch No.: 3

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: C₂₄H₂₉N₇O₂·C₂H₆O₄S

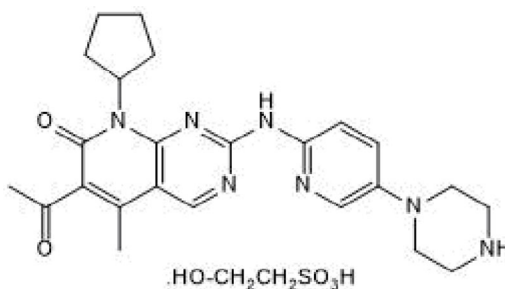
Batch Molecular Weight: 573.66

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 10 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.44	6.15	17.09
Found	54.24	6.17	17.34

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

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Description:

PD 0332991 isethionate is a potent cyclin-dependent kinase 4 (cdk4) and cdk6 inhibitor (IC₅₀ values are 11 nM and 15 nM respectively). Also displays activity at cdk2, cdk5 and cdk9 (IC₅₀ 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:

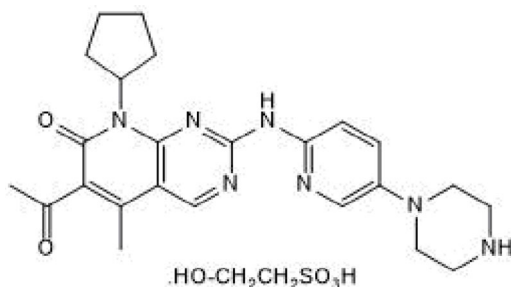
Batch Molecular Formula: C₂₄H₂₉N₇O₂·C₂H₆O₄S

Batch Molecular Weight: 573.66

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: Store 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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