

Product Name: PD 407824

Catalog No.: 2694

Batch No.: 1

CAS Number: 622864-54-4

IUPAC Name: 9-Hydroxy-4-phenyl-pyrrolo[3,4-c]carbazole-1,3(2*H*,6*H*)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₂N₂O₃·¼H₂O

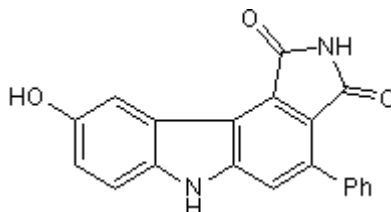
Batch Molecular Weight: 332.82

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.17	3.79	8.42
Found	72.53	3.82	8.14

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

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Description:

Selective inhibitor of checkpoint kinases Chk1 and Wee1 (IC₅₀ values are 47 and 97 nM respectively). Displays selectivity over a range of other protein kinases; IC₅₀ values are 3.4, 3.75, > 5, > 50, > 50 and > 50 µM for PKC, CDK4, other CDKs, c-Src, PDGFR and FGFR respectively.

Physical and Chemical Properties:

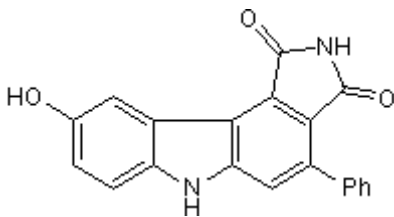
Batch Molecular Formula: C₂₀H₁₂N₂O₃ · ¼ H₂O

Batch Molecular Weight: 332.82

Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 25 mM

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Squire et al (2005) Structure and inhibition of the human cell cycle checkpoint kinase, Wee1A kinase: an atypical tyrosine kinase with a key role in CDK1 regulation. *Structure* **13** 541. PMID: 15837193.

Palmer et al (2006) 4-Phenylpyrrolo[3,4-c]carbazole-1,3(2*H*,6*H*)-dione inhibitors of the checkpoint kinase Wee1. Structure-activity relationships for chromophore modification and phenylring substitutions. *J.Med.Chem.* **49** 4896. PMID: 16884302.

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