

Certificate of Analysis

Print Date: Feb 26th 2024

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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(2H,6H)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{12}N_2O_3.^{1/4}H_2O$

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

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Product Information

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

Description:

PD 407824 is a potent and selective inhibitor of checkpoint kinases Chk1 and Wee1 (IC $_{50}$ values are 47 and 97 nM respectively). Displays selectivity over a range of other protein kinases; IC $_{50}$ values are 3.4, 3.75, > 5, > 50, > 50 and > 50 μ M for PKC, CDK4, other CDKs, c-Src, PDGFR and FGFR respectively. Also sensitizes hESCs to BMP4 to induce differentiation.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₁₂N₂O₃.¹/₄H₂O

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 in lyophilized form. It may appear as a solid, gel or film and 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. *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.

References:

Feng *et al* (2016) Discovery of a small-molecule BMP sensitizer for human embryonic stem cell differentiation. Cell Rep. *15* 2063. PMID: 27210748.

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.

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.

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