# **Screening Libraries**

# **Product** Data Sheet

# PD 407824

Cat. No.: HY-18961 CAS No.: 622864-54-4 Molecular Formula:  $C_{20}H_{12}N_2O_3$ Molecular Weight: 328.32

Checkpoint Kinase (Chk); Wee1 Target:

Pathway: Cell Cycle/DNA Damage

Storage: Powder -20°C 3 years

2 years

-80°C In solvent 2 years

> -20°C 1 year

## **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 250 mg/mL (761.45 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.0458 mL	15.2290 mL	30.4581 mL
	5 mM	0.6092 mL	3.0458 mL	6.0916 mL
	10 mM	0.3046 mL	1.5229 mL	3.0458 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (6.34 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.08 mg/mL (6.34 mM); Clear solution

### **BIOLOGICAL ACTIVITY**

Description	PD 407824 is a checkpoint kinase Chk1 and WEE1 inhibitor with IC $_{50}$ s of 47 and 97 nM, respectively. PD 407824 is a chemical BMP sensitizer and increases the sensitivity of cells to sub-threshold amounts of BMP4 $^{[1][2]}$ .		
IC <sub>50</sub> & Target	Chk1 47 nM (IC <sub>50</sub> )	WEE1 97 nM (IC <sub>50</sub> )	
In Vitro	PD 407824 is sufficient to block CHK1, leading to a significant down-regulation of p21, causing activation of CDK8/9, which in turn causes depletion of SMAD2/3 <sup>[1]</sup> .  PD 407824 is selective for Chk1 and WEE1 over PKC and Cdk4 with IC <sub>50</sub> s of 3.4 μM and 3.75 μM, respectively <sup>[3]</sup> .		

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

#### **REFERENCES**

- [1]. Palmer BD, et al. 4-Phenylpyrrolo[3,4-c]carbazole-1,3(2H,6H)-dione inhibitors of the checkpoint kinase Wee1. Structure-activity relationships for chromophore modification and phenyl ring substitution. J Med Chem. 2006 Aug 10;49(16):4896-911.
- [2]. Feng L, et al. Discovery of a Small-Molecule BMP Sensitizer for Human Embryonic Stem Cell Differentiation. Cell Rep. 2016 May 31;15(9):2063-75.
- [3]. Smaill JB, et al. Synthesis and structure-activity relationships of N-6 substituted analogues of 9-hydroxy-4-phenylpyrrolo[3,4-c]carbazole-1,3(2H,6H)-diones as inhibitors of Wee1 and Chk1 checkpointkinases. Eur J Med Chem. 2008 Jun;43(6):1276-96. Epub 2007 Aug 6.

Caution: Product has not been fully validated for medical applications. For research use only.

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