Certificate of Analysis

Product Name: **PHA 767491 hydrochloride** **Catalog No.: 3140** **Batch No.: 3**

CAS Number: 942425-68-5

IUPAC Name: 1,5,6,7-Tetrahydro-2-(4-pyridinyl)-4*H*-pyrrolo[3,2-*c*]pyridin-4-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{11}N_3O.HCl.2H_2O$

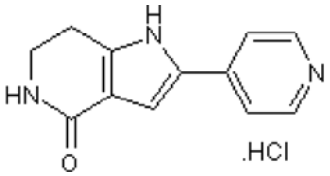
Batch Molecular Weight: 285.73

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.44	5.64	14.71
Found	50.32	5.83	14.52

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Description:

ATP-competitive cyclin-dependent kinase (cdk) inhibitor (reported IC_{50} values are 0.034 - 0.75, 0.24 - 1.2, 0.25 - 1.1 and 0.46 - 1 µM for cdk9, cdk2, cdk1 and cdk5, respectively). Also inhibits mitogen-activated protein kinase-activated protein kinase-2 (MK2; IC_{50} = 171 nM). Prevents initiation of DNA replication. Inhibits cell proliferation in a variety of human cell lines and induces apoptosis in a p53-independent manner in vivo.

Physical and Chemical Properties:

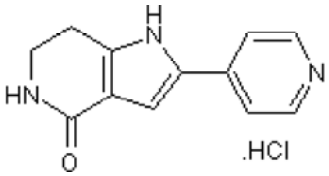
Batch Molecular Formula: $C_{12}H_{11}N_3O.HCl.2H_2O$

Batch Molecular Weight: 285.73

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO to 100 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.

References:

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

Jackson (2008) Stopping replication, at the beginning. Nature Chem.Biol. ***4*** 331.

Montagnoli *et al* (2008) A cdc7 kinase inhibitor restricts initiation of DNA replication and has antitumour activity. Nature Chem.Biol. ***4*** 357.

Anderson *et al* (2007) Pyrrolopyridine inhibitors of mitogen-activated protein kinase-activated protein kinase 2 (MK-2). J.Med.Chem. ***50*** 2647. PMID: 17480064.