

Certificate of Analysis

Print Date: Jan 14th 2016

Batch No.: 1

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Catalog No.: 4569

Product Name: PS 1145 dihydrochloride

CAS Number: 1049743-58-9

IUPAC Name: N-(6-Chloro-9H-pyrido[3,4-b]indol-8-yl)-3-pyridinecarboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{11}CIN_4O.2HCI$

Batch Molecular Weight: 395.67 **Physical Appearance:** Yellow solid

Solubility: DMSO to 5 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.2 \text{ (Chloroform:Methanol [9:1])}$

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 51.6 3.31 14.16 Found 51.26 3.31 13.85



Product Information

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IUPAC Name: N-(6-Chloro-9*H*-pyrido[3,4-*b*]indol-8-yl)-3-pyridinecarboxamide dihydrochloride

Description:

Selective IkB kinase (IKK) inhibitor (IC $_{50}$ = 100 nM). Has no effect on PKA, PKC and CKII activity. Inhibits IkB- α phosphorylation and NFkB activation in HeLa cells. Inhibits NFkB-mediated proinflammatory gene expression in human airway epithelial cells. Enhances TNF- α -induced apoptosis in a multiple myeloma cell line. Attenuates LPS-induced TNF- α production in vivo. Orally active.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₁CIN₄O.2HCI

Batch Molecular Weight: 395.67 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 5 mM with gentle warming

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:

Hideshima *et al* (2002) NF-kappa B as a therapeutic target in multiple myeloma. J.Biol.Chem. **277** 16639. PMID: 11872748. **Castro** *et al* (2003) Novel IKK inhibitors: beta-carbolines. Bioorg.Med.Chem.Lett. **13** 2419. PMID: 12824047.

Newton *et al* (2007) Repression of inflammatory gene expression in human pulmonary epithelial cells by small-molecule IkappaB kinase inhibitors. J.Pharmacol.Exp.Ther. **321** 734. PMID: 17322026.