



Certificate of Analysis

www.tocris.com

Product Name: PKI 166 hydrochloride Catalog No.: 4941 Batch No.: 2

CAS Number: 2230253-82-2

IUPAC Name: 4-[4-[[(1R)-1-Phenylethyl]amino]-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₈N₄O.HCl.H₂O

Batch Molecular Weight: 384.86

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 62.42 5.5 14.56 Found 62.36 5.44 14.52

www.tocris.com/distributors Tel:+1 612 379 2956



Product Information

Print Date: Jan 27th 2020

www.tocris.com

Batch No.: 2

Product Name: PKI 166 hydrochloride

CAS Number: 2230253-82-2

IUPAC Name: 4-[4-[[(1R)-1-Phenylethyl]amino]-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenol hydrochloride

Description:

Potent EGFR-kinase inhibitor ($IC_{50} = 0.7$ nM). Displays >3000-fold selectivity against a panel of serine/threonine kinases. Reduces metastasis and angiogenesis in a mouse model of pancreatic cancer. Antihypertensive and orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₁₈N₄O.HCI.H₂O

Batch Molecular Weight: 384.86 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 4941

Solubility & Usage Info:

DMSO to 100 mM ethanol to 50 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:

Ulu et al (2013) Epidermal growth factor receptor inhibitor PKI-166 governs cardiovascular protection without beneficial effects on the kidney in hypertensive 5/6 nephrectomized rats. J.Pharmacol.Exp.Ther. **345** 393. PMID: 23528611.

Kaspersen et al (2012) Activity of 6-aryl-pyrrolo[2,3-d]pyrimidine-4-amines to Tetrahymena. Bioorg. Chem. 44 35. PMID: 22832269.

Bruns et al (2000) Blockade of the epidermal growth factor receptor signaling by a novel tyrosine kinase inhibitor leads to apoptosis of endothelial cells and therapy of human pancreatic carcinoma. Cancer Res. **60** 2926. PMID: 10850439.

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