

Print Date: Jan 14th 2016

Certificate of Analysis www.tocris.com

Product Name: PF 06465469 Catalog No.: 4710 Batch No.: 1

CAS Number: 1407966-77-1

IUPAC Name: (R)-3-(1-(1-Acryloylpiperidin-3-yl)-4-amino-1H-pyrazolo[3,4-d]pyrimidin-3-yl)-N-(3-methyl-4-(1-methylethyl))

benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{33}N_7O_2.^{3}H_2O$

Batch Molecular Weight: 537.14

Physical Appearance: Off-white solid

Solubility: DMSO to 5 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 95.5% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.08 6.47 18.25 Found 67.15 6.38 17.96

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



Product Information

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Description:

Potent inhibitor of interleukin-2 inducible T cell kinase (ITK) (IC $_{50}$ = 2 nM). Also exhibits inhibitory activity against Bruton's tyrosine kinase (BTK) (IC $_{50}$ = 2 nM). Displays nanomolar potencies in a cell-based IP1 assay and human whole blood assay (IC $_{50}$ values are 31 and 48 nM respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{30}H_{33}N_7O_2$. $^{3}_4H_2O$

Batch Molecular Weight: 537.14 Physical Appearance: Off-white solid

Minimum Purity: >95%

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:

Zapf *et al* (2012) Covalent inhibitors of interleukin-2 inducible T cell kinase (Itk) with nanomolar potency in a whole-blood assay. J.Med.Chem. *55* 10047. PMID: 23098091.

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