



Certificate of Analysis

www.tocris.com

Product Name: (R)-DRF053 dihydrochloride Catalog No.: 3610 Batch No.: 2

CAS Number: 1241675-76-2

IUPAC Name: 2-[[9-(1-Methylethyl)-6-[[3-(2-pyridinyl)phenyl]amino]-9*H*-purin-2-yl]amino]-1-butanol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{27}N_7O.2HCI._{34}H_2O$

Batch Molecular Weight:503.94Physical Appearance:yellow solidSolubility:water to 100 mM

DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Chloroform:Methanol:Ammonia soln. [9:1:5])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.82 6.1 19.42 Found 54.67 5.99 19.33

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





Print Date: Feb 19th 2014

Batch No.: 2

TOCRIS

www.tocris.com

Product Name: (R)-DRF053 dihydrochloride

CAS Number: 1241675-76-2

IUPAC Name: 2-[[9-(1-Methylethyl)-6-[[3-(2-pyridinyl)phenyl]amino]-9*H*-purin-2-yl]amino]-1-butanol dihydrochloride

Description:

Potent, ATP-competitive inhibitor of cyclin-dependent kinase (cdk) and casein kinase 1 (CK1) (IC $_{50}$ values are 220, 80 and 14 nM for cdk1/cyclin B, cdk5/p25 and CK1 respectively). Selective over GSK-3 $\alpha\beta$ (IC $_{50}$ = 4.1 μ M). Also shown to inhibit amyloid- β production in N2A-APP $_{695}$ cells.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{23}H_{27}N_7O.2HCI.34H_2O$

Batch Molecular Weight: 503.94 Physical Appearance: yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

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).

Catalog No.: 3610

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:

Oumata et al (2008) Roscovitine-derived, dual-specificity inhibitors of cyclin-dependent kinases and casein kinases 1. J.Med.Chem. **51** 522.

