

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]-9H-purin-2-yl]amino]-1-butanol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₇N₇O.2HCl.¾H₂O

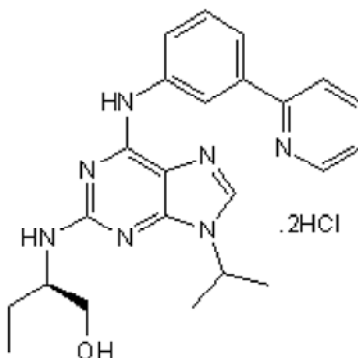
Batch Molecular Weight: 503.94

Physical Appearance: Yellow solid

Solubility: 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

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Description:

Potent casein kinase 1 (CK1) inhibitor (IC_{50} = 14 nM). Also an ATP-competitive cyclin-dependent kinase (cdk) inhibitor (IC_{50} values are 0.093 - 0.29, 0.21 and 0.82 μ M for cdk2, cdk5 and cdk7, respectively). Shown to inhibit amyloid- β production in N2A-APP695 cells.

Physical and Chemical Properties:

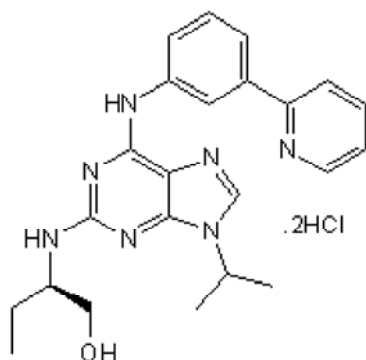
Batch Molecular Formula: $C_{23}H_{27}N_7O \cdot 2HCl \cdot \frac{3}{4}H_2O$

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).

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.

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

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