TOCRIS a bio-techne brand

Print Date: Nov 10th 2021

Certificate of Analysis

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Product Name: (*R*)-CR8 **Catalog No.: 3605** **Batch No.: 2**

CAS Number: 1786438-30-9

IUPAC Name: (2*R*)-2-[[9-(Methylethyl)-6-[[[4-(2-pyridinyl)phenyl]methyl]amino]-9*H*-purin-2-yl]amino]-1-butanol trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{29}N_7O.3HCl.H_2O$

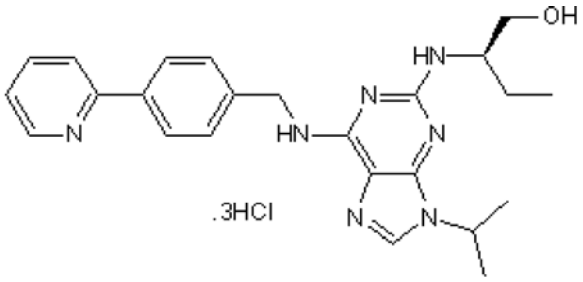
Batch Molecular Weight: 558.94

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

Chiral HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	51.57	6.13	17.54	19.03
Found	51.3	6.37	17.44	18.74

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Description:

(R)-CR8 is a cyclin dependent kinase (cdk) inhibitor (reported IC_{50} values are 0.036 - 0.07, 0.09 - 0.8, 0.13 - 0.68, 0.18 - 1 and >1 µM for cdk2, cdk1, cdk5, cdk9 and cdk7, respectively). Also inhibits casein kinase 1 (CK1; IC_{50} = 0.6 µM). Acts as molecular glue; forms a complex between CDK12-cyclin K and the CUL4 adapter protein DDB1 resulting in ubiquination and degradation of cyclin K.

Physical and Chemical Properties:

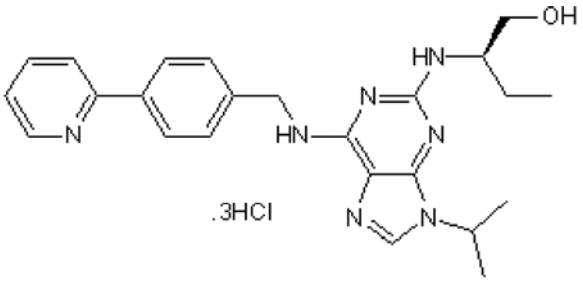
Batch Molecular Formula: $C_{24}H_{29}N_7O.3HCl.H_2O$

Batch Molecular Weight: 558.94

Physical Appearance: White solid

Minimum Purity: ≥99%

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:

Słabicki *et al* (2020) The CDK inhibitor CR8 acts as a molecular glue degrader that depletes cyclin K. Nature ***585*** 293. PMID: 32494016.

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*** 5229. PMID: 18698753.