TOCRIS
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Print Date: Jul 23rd 2020

Certificate of Analysis

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Product Name: **K 03861** **Catalog No.: 6789** **Batch No.: 1**

CAS Number: 853299-07-7

IUPAC Name: *N*-[4-[(2-Amino-4-pyrimidinyl)oxy]phenyl]-*N'*-[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{26}F_3N_7O_2.¼H_2O$

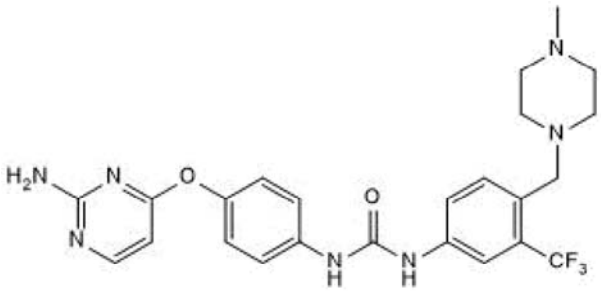
Batch Molecular Weight: 506.01

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.97	5.28	19.38
Found	57.03	5.27	19.21

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Description:

Potent Cdk2 inhibitor (K_d values are 9.7, 15.4, 18.6 and 50 nM at Cdk2 (C118L/A144C), Cdk2 (A144C), Cdk2 (C118L), and Cdk (WT) respectively. Competes with cyclin binding to inhibit Cdk2 kinase activity in vitro.

Physical and Chemical Properties:

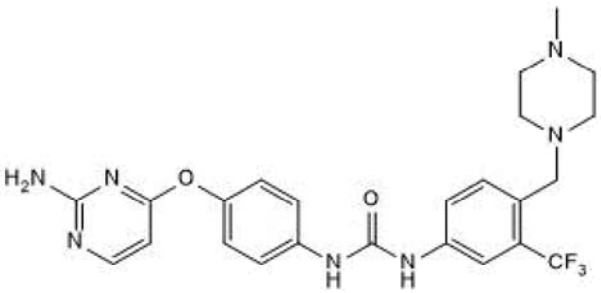
Batch Molecular Formula: $C_{24}H_{26}F_3N_7O_2.¼H_2O$

Batch Molecular Weight: 506.01

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM
ethanol 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:

Song *et al* (2017) NEUROG1 regulates CDK2 to promote proliferation in otic progenitors Stem Cell Reports ***9*** 1516. PMID: 29033307.

Alexander *et al* (2015) Type II inhibitors targeting Cdk2 ACS.Chem.Biol ***10*** 2116. PMID: 26158339.