Certificate of Analysis

Product Name: **KRCA 0008** **Catalog No.: 5098** **Batch No.: 1**

CAS Number: 1472795-20-2

IUPAC Name: 1,1'-[(5-Chloro-2,4-pyrimidinediyl)bis[imino(3-methoxy-4,1-phenylene)-4,1-piperazinediyl]]bisethanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{37}ClN_8O_4.¾H_2O$

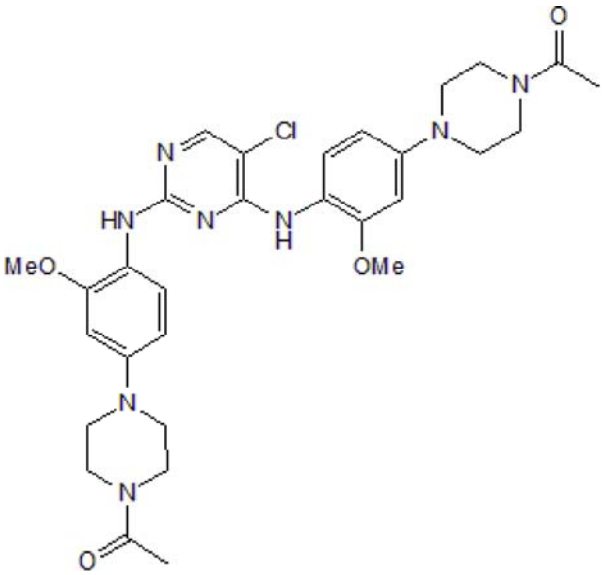
Batch Molecular Weight: 622.63

Physical Appearance: Pale brown solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.6 (Chloroform:Methanol [95:5])

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.87	6.23	18
Found	57.68	6.1	18.07

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Product Information

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Description:

Potent Ack1 and anaplastic lymphoma kinase (ALK) dual inhibitor (IC_{50} values are 4 and 12 nM respectively). Inhibits lung cancer H3122 cell proliferation (IC_{50} = 80 nM). Attenuates H3122 cell xenograft tumor growth in mice. Orally bioavailable.

Physical and Chemical Properties:

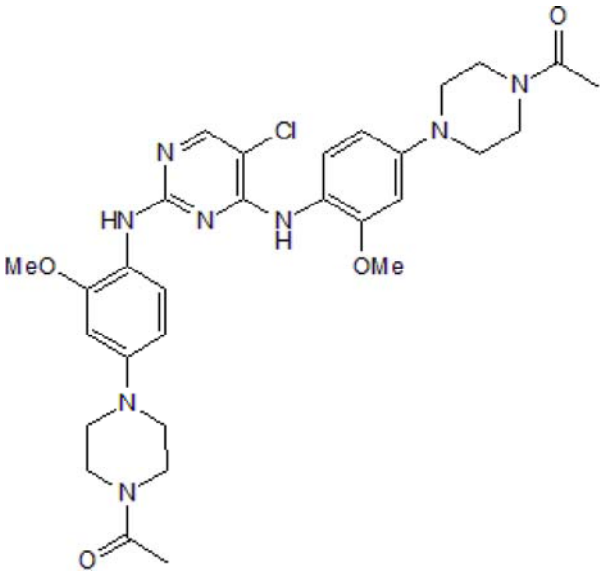
Batch Molecular Formula: $C_{30}H_{37}ClN_8O_4.¾H_2O$

Batch Molecular Weight: 622.63

Physical Appearance: Pale brown solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM
DMSO to 100 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:

Lee *et al* (2014) ALK inhibitors of bis-ortho-alkoxy-para-piperazinesubstituted-pyrimidines and -triazines for cancer treatment. Arch.Pharm.Res. ***37*** 1130. PMID: 24446111.

Park *et al* (2013) Novel bis-ortho-alkoxy-para-piperazinesubstituted-2,4-dianilinopyrimidines (KRCA-0008) as potent and selective ALK inhibitors for anticancer treatment. Bioorg.Med.Chem.Lett. ***23*** 6192. PMID: 24095090.

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