



Certificate of Analysis

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Product Name: Bosutinib Catalog No.: 4361 Batch No.: 1

CAS Number: 380843-75-4

Batch Molecular Structure:

IUPAC Name: 4-[(2,4-Dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-methyl-1-piperazinyl)propoxy]-3-

quinolinecarbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{29}CI_2N_5O_3$. ½ H_2O

Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM ethanol to 25 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.89 5.61 12.98 Found 57.72 5.81 12.95



Product Information

Print Date: Feb 7th 2013

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quinolinecarbonitrile

Description:

Dual inhibitor of Abl and Src kinases ($IC_{50} = 1.2$ nM for Src in an enzymatic assay). Displays antiproliferative activity against chronic myelogenous leukemia (CML) cells and decreases the motility and invasion of breast cancer cell lines. Also exhibits potent antiproliferative activity in anchorage-independent, Src-transformed rat fibroblasts ($IC_{50} = 100$ nM). Displays selectivity for Src over non-Src family kinases such as growth factor receptor tyrosine kinases.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₉Cl₂N₅O₃.½H₂O

Batch Molecular Weight: 539.46 Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Useage Info:

Soluble to 100 mM in DMSO and to 25 mM in ethanol

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:

Boschelli et al (2001) Optimization of 4-phenylamino-3-quinolinecarbonitriles as potent inhibitors of Src kinase activity. J.Med.Chem. **44** 3965. PMID: 11689083.

Golas *et al* (2003) SKI-606, a 4-anilino-3-quinolinecarbonitrile dual inhibitor of Src and Abl kinases, is a potent antiproliferative agent against chronic myelogenous leukemia cells in culture and causes regression of K562 xenografts in nude mice. Cancer Res. *63* 375. PMID: 12543790.

Golas et al (2005) SKI-606, a Src/Abl inhibitor with in vivo activity in colon tumor xenograft models. Cancer Res. 65 5358. PMID: 15958584.

Vultur *et al* (2008) SKI-606 (bosutinib), a novel Src kinase inhibitor, suppresses migration and invasion of human breast cancer cells. Mol.Cancer.Ther. **7** 1185. PMID: 18483306.

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