

Product Name: Bosutinib

Catalog No.: 4361

Batch No.: 1

CAS Number: 380843-75-4

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: C₂₆H₂₉Cl₂N₅O₃ · ½H₂O

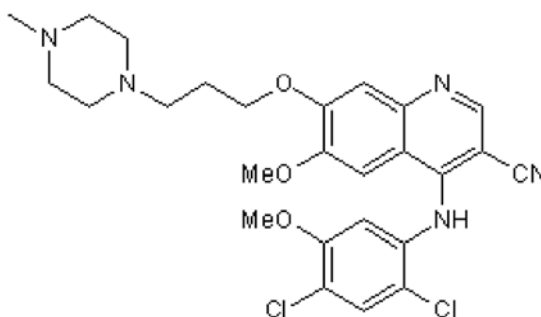
Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



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

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Dual inhibitor of Abl and Src kinases (IC₅₀ = 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 (IC₅₀ = 100 nM). Displays selectivity for Src over non-Src family kinases such as growth factor receptor tyrosine kinases.

Physical and Chemical Properties:

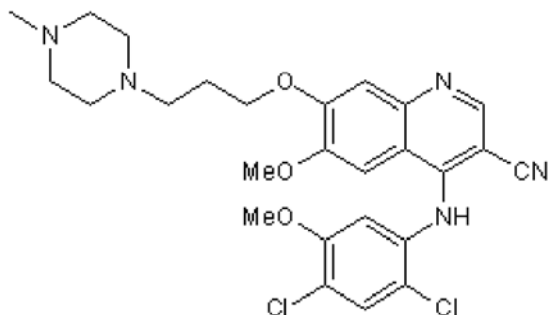
Batch Molecular Formula: C₂₆H₂₉Cl₂N₅O₃·½H₂O

Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage 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.

Congratulations on your purchase of Bosutinib, sold under license from Pfizer, Inc. If your research with Bosutinib results in a new discovery (e.g., new uses, new combinations, etc.) Pfizer is interested in discussing these discoveries with you. Also note that Pfizer has a Compound Transfer Program that provides a free sample of any Pfizer product at www.pfizer.com/research/rd_works/compound_transfer_program.jsp

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