

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: $C_{26}H_{29}Cl_2N_5O_3 \cdot \frac{1}{2}H_2O$

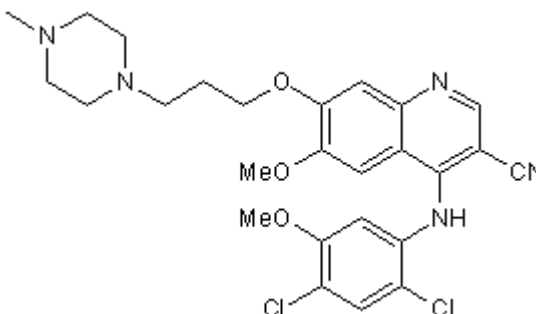
Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

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

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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:

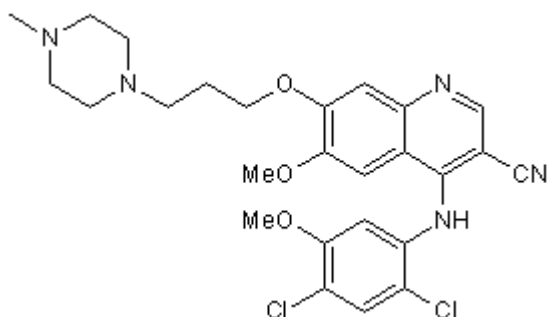
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Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



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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