

Product Name: Dasatinib

Catalog No.: 6793

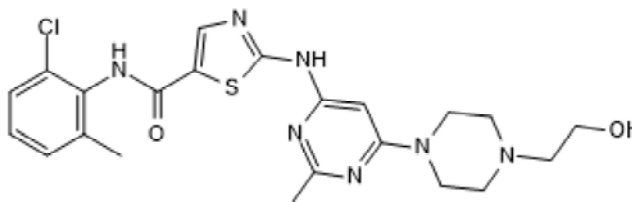
Batch No.: 1

CAS Number: 302962-49-8

IUPAC Name: *N*-(2-Chloro-6-methylphenyl)-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl]-2-methyl-4-pyrimidinyl]amino]-5-thiazolecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₆ClN₇O₂S
Batch Molecular Weight: 488.01
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.15	5.37	20.09
Found	54.01	5.34	19.98

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

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Description:

Highly potent pan-Src/Bcr-Abl inhibitor (K_i values are 16 and 30 pM, respectively). Inhibits Bcr-Abl, Src, Lck, Fyn, c-kit and Yes with IC_{50} values in the subnanomolar range. Inhibits proliferation of tumor cells in vitro and exhibits anticancer activity in vivo in a mouse chronic myelogenous leukemia (CML) xenograft model.

Physical and Chemical Properties:

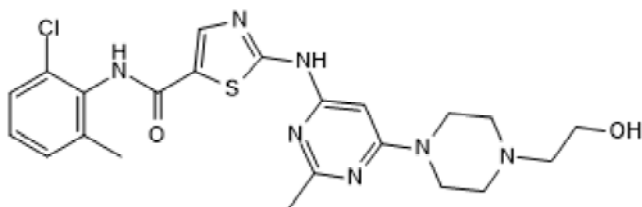
Batch Molecular Formula: $C_{22}H_{26}ClN_7O_2S$

Batch Molecular Weight: 488.01

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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:

Das et al (2006) 2-aminothiazole as a novel kinase inhibitor template. Structure-activity relationship studies toward the discovery of *N*-(2-chloro-6-methylphenyl)-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl]-2-methyl-4-pyrimidinyl]amino]-1,3-thiazole-5-carboxamide (dasatinib, BMS-354825) as a potent *pan*-Src kinase inhibitor. *J.Med.Chem.* **49** 6819. PMID: 17154512.

Lombardo et al (2004) Discovery of *N*-(2-chloro-6-methylphenyl)-2-(6-(4-(2-hydroxyethyl)piperazin-1-yl)-2-methylpyrimidin-4-ylamino)thiazole-5-carboxamide (BMS-354825), a dual Src/Abl kinase inhibitor with potent antitumor activity in preclinical assays. *J.Med.Chem.* **47** 6658. PMID: 15615512.

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