

Product Name: Dasatinib

Catalog No.: 6793

Batch No.: 2

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.H₂O

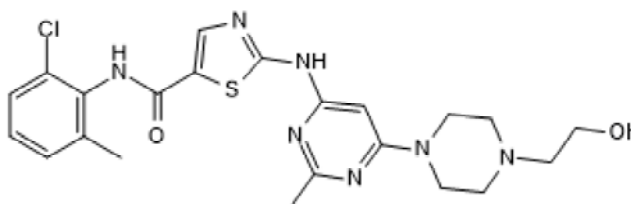
Batch Molecular Weight: 506.03

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°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	52.22	5.58	19.38
Found	52.08	5.61	19.38

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 μM , 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. Inhibits replication of SARS-CoV and MERS-CoV in vitro (EC_{50} values are 2.1 and 5.5 μM , respectively).

Physical and Chemical Properties:

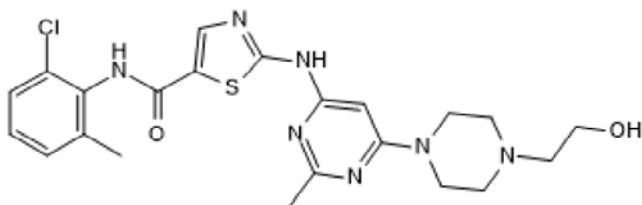
Batch Molecular Formula: $\text{C}_{22}\text{H}_{26}\text{ClN}_7\text{O}_2\text{S}\cdot\text{H}_2\text{O}$

Batch Molecular Weight: 506.03

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Dyall et al (2014) Repurposing of clinically developed drugs for treatment of Middle East Respiratory Syndrome coronavirus infection. *Antimicrob. Agents Chemother.* **58** 4885. PMID: 24841273.

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. *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.

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 $45\text{-}60^\circ\text{C}$ 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.

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