Print Date: Feb 6th 2014

Certificate of Analysis

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Product Name: BMS 599626 dihydrochloride **Catalog No.: 5022** **Batch No.: 1**

IUPAC Name: (3*S*)-3-Morpholinylmethyl-[4-[[1-[(3-fluorophenyl)methyl]-1*H*-indazol-5-yl]amino]-5-methylpyrrolo[2,1-*f*][1,2,4] triazin-6-yl]-carbamate dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{27}FN_8O_3.2HCl.1¾H_2O$

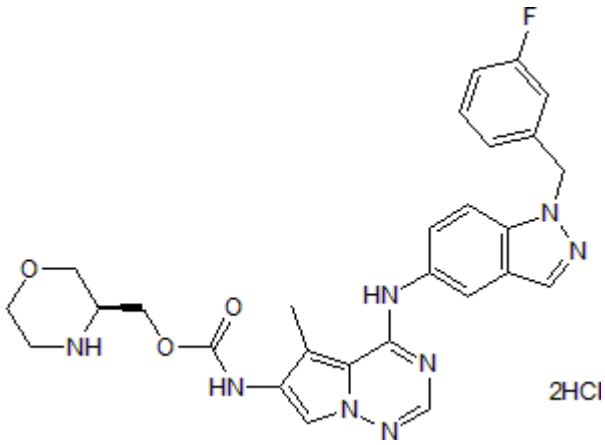
Batch Molecular Weight: 635

Physical Appearance: White solid

Solubility: water to 5 mM with gentle warming
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.07	5.16	17.65
Found	51.08	5.02	17.41

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Description:

Potent and selective EGFR and ErbB2 inhibitor (IC_{50} values are 22 nM and 32 nM respectively). Also inhibits HER4 (IC_{50} = 190 nM). Inhibits EGFR and ErbB2 with 100-fold greater potency than MEK and Lck. Antiproliferative agent in vitro and anti-tumorigenic agent in vivo. Orally bioavailable.

Physical and Chemical Properties:

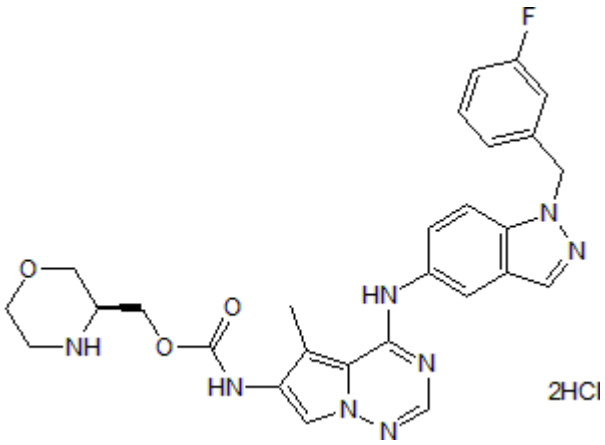
Batch Molecular Formula: $C_{27}H_{27}FN_8O_3.2HCl.1¾H_2O$

Batch Molecular Weight: 635

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 5 mM with gentle warming
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:

Wong *et al* (2006) Preclinical antitumor activity of BMS-599626, a pan-HER kinase inhibitor that inhibits HER1/HER2 homodimer and heterodimer signaling. Clin.Cancer Res. ***12*** 6186. PMID: 17062696.

Gavai *et al* (2009) Discovery and preclinical evaluation of [4-[[1-(3-fluorophenyl)methyl]-1*H*-indazol-5-ylamino]-5-methylpyrrolo [2,1-*f*][1,2,4]triazin-6-yl]carbamic acid, (3*S*)-3-morpholinylmethyl ester (BMS-599626), a selective and orally efficacious inhibitor of human epidermal growth factor receptor 1 and 2 kinases. J.Med.Chem. ***52*** 6527. PMID: 19821562.