

**Product Name:** BMS 599626 dihydrochloride

**Catalog No.:** 5022

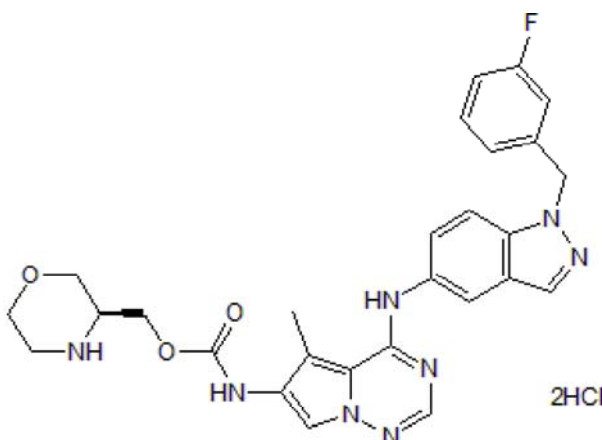
**Batch No.:** 1

CAS Number: 1781932-33-9

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

<b>Batch Molecular Formula:</b>	C <sub>27</sub> H <sub>27</sub> FN <sub>8</sub> O <sub>3</sub> ·2HCl·1 <sup>3</sup> / <sub>4</sub> H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	635
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	water to 5 mM with gentle warming DMSO to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 98.9% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	
	Carbon Hydrogen Nitrogen
Theoretical	51.07    5.16    17.65
Found	51.08    5.02    17.41

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

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**Description:**

Potent and selective EGFR and ErbB2 inhibitor (IC<sub>50</sub> values are 22 nM and 32 nM respectively). Also inhibits HER4 (IC<sub>50</sub> = 190 nM). Inhibits EGFR and ErbB2 with 100-fold greater potency than MEK and Lck. Antiproliferative agent in vitro and antitumorigenic agent in vivo. Orally bioavailable.

**Physical and Chemical Properties:**

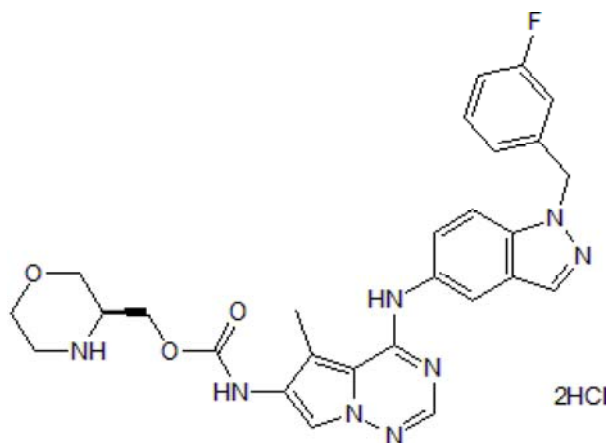
Batch Molecular Formula: C<sub>27</sub>H<sub>27</sub>FN<sub>8</sub>O<sub>3</sub>·2HCl·1¼H<sub>2</sub>O

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:**

**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 J. Med. Chem. **52** 6527. PMID: 19821562.

**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.

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