

Certificate of Analysis

Product Name: Canertinib dihydrochloride

Catalog No.: 5916

Batch No.: 1

CAS Number: 289499-45-2

IUPAC Name: *N*-[4-[(3-Chloro-4-fluorophenyl)amino]-7-[3-(4-morpholinyl)propoxy]-6-quinazoliny]-2-propenamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₅ClFN₅O₃·2HCl·2½H₂O

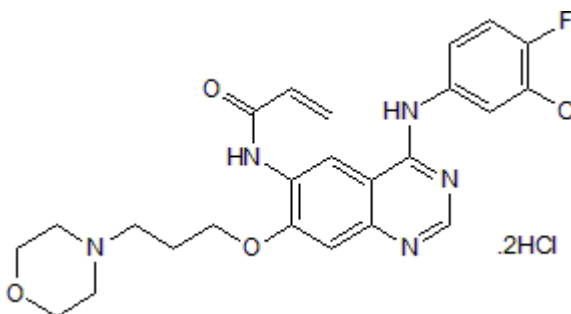
Batch Molecular Weight: 603.9

Physical Appearance: Yellow solid

Solubility: water to 20 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.73	5.34	11.6
Found	47.4	5.42	11.44

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

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Description:

Potent EGFR kinase inhibitor ($IC_{50} = 7.4$ nM). Blocks autophosphorylation of erbB2. Inhibits growth of A431 tumor xenografts in mice. Cell permeable.

Physical and Chemical Properties:

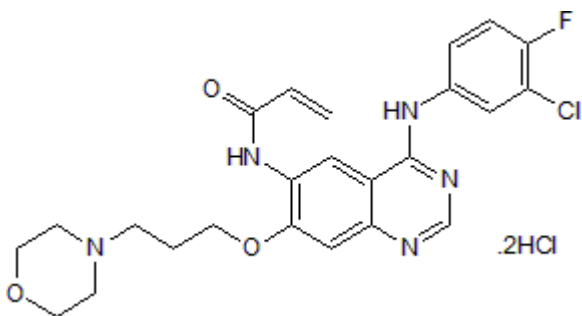
Batch Molecular Formula: $C_{24}H_{25}ClFN_5O_3 \cdot 2HCl \cdot 2\frac{1}{2}H_2O$

Batch Molecular Weight: 603.9

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 20 mM
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:

Small *et al* (2000) Tyrosine kinase inhibitors. 17. Irreversible inhibitors of the epidermal growth factor receptor: 4-(phenylamino)quinazoline- and 4-(phenylamino)pyrido[3,2-d]pyrimidine-6-acrylamides bearing additional solubilizing functions. *J.Med.Chem.* **43** 1380. PMID: 10753475.

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