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Print Date: Jul 23rd 2019

Certificate of Analysis

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Product Name: **BIBU 1361 dihydrochloride** **Catalog No.: 2417** **Batch No.: 2**

CAS Number: 1643609-75-9

IUPAC Name: *N*-(3-Chloro-4-fluorophenyl)-6-[4-[(diethylamino)methyl]-1-piperidinyl]-pyrimido[5,4-*d*]pyrimidin-4-amine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C22H27ClFN7.2HCl

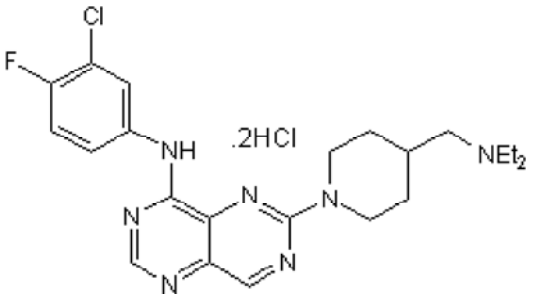
Batch Molecular Weight: 516.87

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 25 mM
ethanol to 5 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.52 (Chloroform:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows >97.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.12	5.65	18.96
Found	50.82	5.65	18.94

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

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Product Information

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Description:

Potent inhibitor of epidermal growth factor receptor (EGFR) tyrosine kinase (IC_{50} = 3 nM). Displays ~ 100-fold lower potency against ErbB2 (IC_{50} = 290 nM) and is selective over a range of other related tyrosine kinases (IC_{50} > 10 µM). Blocks downstream EGFR signaling events such as MAPKK/MAPK activation. Oral administration inhibits growth of established human xenografts in athymic mice.

Physical and Chemical Properties:

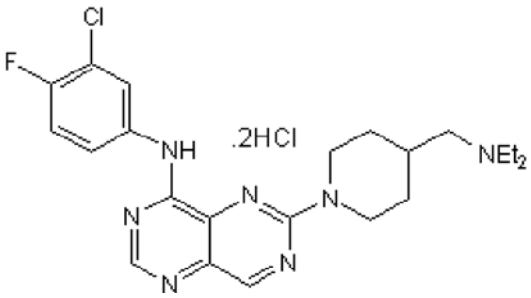
Batch Molecular Formula: $C_{22}H_{27}ClFN_7.2HCl$

Batch Molecular Weight: 516.87

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM
DMSO to 25 mM
ethanol to 5 mM

When purchsed as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Solca *et al* (2004) Inhibition of epidermal growth factor receptor activity by two pyrimidopyrimidine derivatives. J.Pharmacol.Exp.Ther. ***311*** 502. PMID: 15199094.