

Certificate of Analysis

www.tocris.com

Product Name: BIBX 1382 dihydrochloride

Catalog No.: 2416

Batch No.: 1

CAS Number: 1216920-18-1

IUPAC Name: *N*⁸-(3-Chloro-4-fluorophenyl)-*N*²-(1-methyl-4-piperidiny)-pyrimido[5,4-*d*]pyrimidine-2,8-diamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₉ClF₇N₇.2HCl.2H₂O

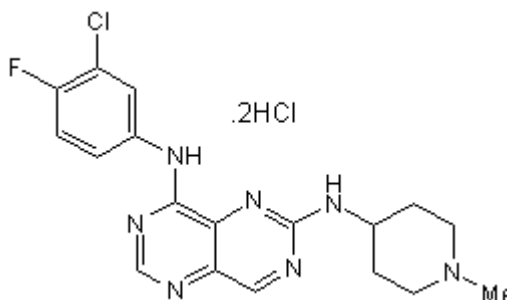
Batch Molecular Weight: 496.8

Physical Appearance: Yellow solid

Solubility: water to 50 mM
DMSO to 50 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 97.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 43.52 5.07 19.74

Found 43.72 5.04 19.38

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

Product Information

www.tocris.com

Product Name: BIBX 1382 dihydrochloride

Catalog No.: 2416

Batch No.: 1

CAS Number: 1216920-18-1

IUPAC Name: *N*⁸-(3-Chloro-4-fluorophenyl)-*N*²-(1-methyl-4-piperidiny)-pyrimido[5,4-*d*]pyrimidine-2,8-diamine dihydrochloride

Description:

Potent, selective inhibitor of epidermal growth factor receptor (EGFR) tyrosine kinase (IC_{50} = 3 nM). Displays > 1000-fold lower potency against ErbB2 (IC_{50} = 3.4 μ M) and a range of other related tyrosine kinases (IC_{50} > 10 μ M). Oral administration inhibits growth of established human xenografts in athymic mice.

Physical and Chemical Properties:

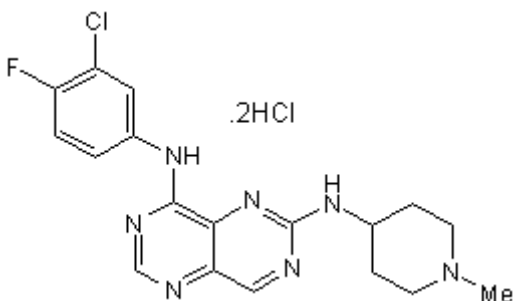
Batch Molecular Formula: $C_{18}H_{19}ClF_2N_7 \cdot 2HCl \cdot 2H_2O$

Batch Molecular Weight: 496.8

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 50 mM

DMSO to 50 mM

When purchased 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:

Dittrich et al (2002) Phase I and pharmacokinetic study of BIBX1382 BS, an epidermal growth factor receptor (EGFR) inhibitor, given in a continuous daily oral administration. *Eur.J.Cancer* **38** 1072. PMID: 12008195.

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

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956