

Certificate of Analysis

Print Date: Sep 3rd 2018

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Product Name: Pelitinib Catalog No.: 6349 Batch No.: 1

CAS Number: 257933-82-7

IUPAC Name: (2E)-N-[4-[(3-Chloro-4-fluorophenyl)amino]-3-cyano-7-ethoxy-6-quinolinyl]-4-(dimethylamino)-2-butenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₃CIFN₅O₂.½H₂O

Batch Molecular Weight:476.93Physical Appearance:Beige solidSolubility:DMSO to 50 mMStorage:Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Dichloromethane:Methanol [1:1])

HPLC: Shows 97.3% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.44 5.07 14.68 Found 60.21 5.05 14.58

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



Product Information

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Description:

Potent irreversible EGFR inhibitor (IC_{50} = 20-80 nM). Selective for EGFR over Src, MEK/ERK, erbB2, Raf, c-Met and Cdk4 (IC_{50} values are 282, 800, 1255, 3353, 4100 and >20,000). Inhibits the growth of tumors overexpressing EGFR in vivo. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C24H23CIFN5O2.12H2O

Batch Molecular Weight: 476.93 Physical Appearance: Beige solid

Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 50 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc

References:

Hegedüs (2012) Interaction of the EGFR inhibitors gefitinib, vandetanib, pelitinib and neratinib with the ABCG2 multidrug transporter: Implications for the emergence and reversal of cancer drug resistance Biochem. Pharmacol. **84** 260. PMID: 22548830.

Tyner *et al* (2006) Blocking airway mucous cell metaplasia by inhibiting EGFR antiapoptosis and IL-13 transdifferentiation signals. J.Clin.Invest. *116* 309. PMID: 16453019.

Nunes *et al* (2004) Phosphorylation of extracellular signal-regulated kinase 1 and 2, protein kinase B, and signal transducer and activator of transcription 3 are differently inhibited by an epidermal growth factor receptor inhibitor, EKB-569, in tumor cells and normal human keratinocytes. Mol.Cancer Ther. **3** 21. PMID: 14749472.

Torrance et al (2000) Combinatorial chemoprevention of intestinal neoplasia. Nat.Med. 6 1024. PMID: 10973323.