

Product Name: AEE 788

Catalog No.: 5318

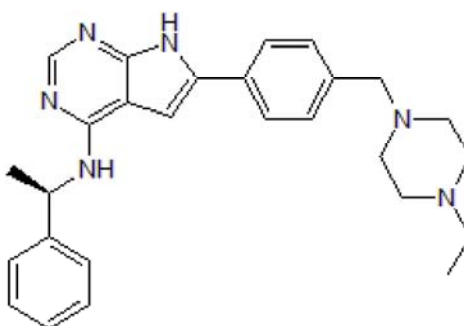
Batch No.: 1

CAS Number: 497839-62-0

IUPAC Name: 6-[4-[(4-Ethyl-1-piperazinyl)methyl]phenyl]-N-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₂N₆·¼H₂O
Batch Molecular Weight: 445.08
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.86	7.36	18.88
Found	72.69	7.21	18.78

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

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Description:

Potent EGFR and VEGFR inhibitor (IC₅₀ values are 2, 6, 59, 77, 160 and 330 nM for EGFR, ErbB2, VEGFR-1, VEGFR-2, ErbB4 and VEGFR-3 respectively). Also inhibits c-Abl, c-Fms and c-Src (IC₅₀ values are 52, 60 and 61 nM respectively). Inhibits proliferation of EGFR and ErbB2 overexpressing cancer cell lines in vitro. Inhibits tumor xenograft growth and VEGF-induced angiogenesis in mice. Orally active.

Physical and Chemical Properties:

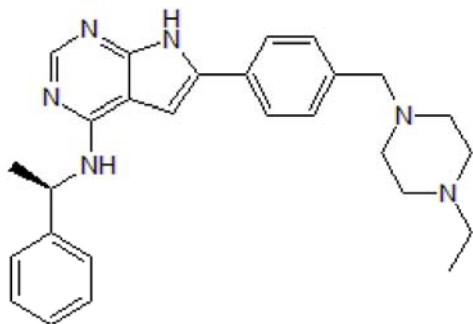
Batch Molecular Formula: C₂₇H₃₂N₆·¼H₂O

Batch Molecular Weight: 445.08

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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:

Yokoi et al (2005) Dual inhibition of epidermal growth factor receptor and vascular endothelial growth factor receptor phosphorylation by AEE788 reduces growth and metastasis of human colon carcinoma in an orthotopic nude mouse model. *Cancer Res.* **65** 3716. PMID: 15867367.

Traxler et al (2004) AEE788: a dual family epidermal growth factor receptor/ErbB2 and vascular endothelial growth factor receptor tyrosine kinase inhibitor with antitumor and antiangiogenic activity. *Cancer Res.* **64** 4931. PMID: 15256466.

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