

Product Name: AV 412

Catalog No.: 4397

Batch No.: 1

CAS Number: 451492-95-8

IUPAC Name: *N*-[4-[(3-Chloro-4-fluorophenyl)amino]-7-[3-methyl-3-(4-methyl-1-piperazinyl)-1-butyn-1-yl]-6-quinazoliny]-2-propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₈ClFN₆O.H₂O

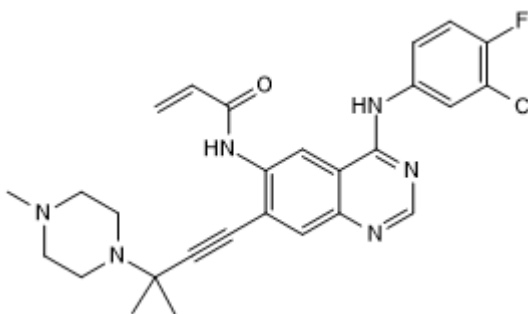
Batch Molecular Weight: 525.02

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
1eq. HCl to 20 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.28 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

HPLC: Shows >99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.77	5.76	16.01
Found	61.92	5.69	16.18

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Description:

Potent inhibitor of EGFR, ErbB2 and Abl receptor tyrosine kinases (IC₅₀ values are 0.5-2, 19 and 41 nM, respectively). Also weak inhibitor of FLT1 and Src. Inhibits EGFR and ErbB2 autophosphorylation in vitro in NSCLC and T-47D breast cancer cell lines, respectively. Inhibits tumor growth of EGFR-overexpressing A431 and ErbB2 overexpressing BT-474 tumor xenografts in mice.

Physical and Chemical Properties:

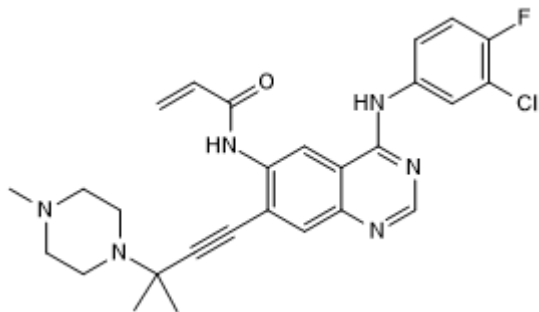
Batch Molecular Formula: C₂₇H₂₈ClFN₆O.H₂O

Batch Molecular Weight: 525.02

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Suzuki et al (2009) Antitumor activity of a dual epidermal growth factor receptor and ErbB2 kinase inhibitor MP-412 (AV-412) in mouse xenograft models. *Cancer Sci.* **100** 1526. PMID: 19459856 .

Suzuki et al (2007) Pharmacological characterization of MP-412 (AV-412), a dual epidermal growth factor receptor and ErbB2 tyrosine kinase inhibitor. *Cancer Sci.* **98** 1977. PMID: 17888033 .

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 20 mM

ethanol 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.

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