

Product Name: TAK 165

Catalog No.: 3599

Batch No.: 2

CAS Number: 366017-09-6

IUPAC Name: 1-[4-[4-[[2-[(1*E*)-2-[4-(trifluoromethyl)phenyl]ethenyl]-4-oxazolyl]methoxy]phenyl]butyl]-1*H*-1,2,3-triazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₃F₃N₄O₂·¼H₂O

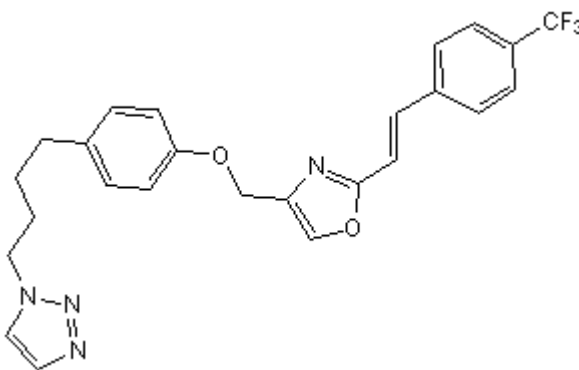
Batch Molecular Weight: 472.97

Physical Appearance: Off White solid

Solubility: DMSO to 75 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.49	5.01	11.85
Found	63.38	4.85	11.81

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

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Description:

Potent, irreversible human epithelial growth factor receptor 2 (ErbB2) inhibitor (IC₅₀ = 6 nM) that displays > 4000-fold selectivity over EGFR, FGFR, PDGFR, JAK1 and Src. Exhibits potent antiproliferative effects in ErbB2-overexpressing cancer cell lines (IC₅₀ = 5 nM in BT474 breast cancer cells) and significantly inhibits bladder, breast and prostate cancer xenograft growth in vivo.

Physical and Chemical Properties:

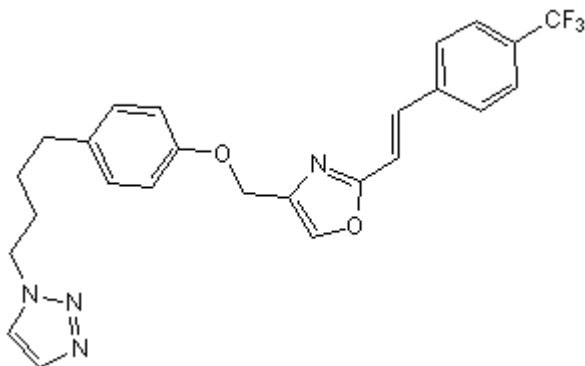
Batch Molecular Formula: C₂₅H₂₃F₃N₄O₂·¼H₂O

Batch Molecular Weight: 472.97

Physical Appearance: Off White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Spector et al (2007) Small molecule HER-2 tyrosine kinase inhibitors. *Breast Cancer Res.* **9** 205.

Nagasawa et al (2006) Novel HER2 selective tyrosine kinase inhibitor, TAK-165, inhibits bladder, kidney and androgen-independent prostate cancer *in vitro* and *in vivo*. *Int.J.Urol.* **13** 585.

Sridhar et al (2003) Inhibitors of epidermal-growth-factor receptors: a review of clinical research with a focus on non-small-cell lung cancer. *Lancet Oncol.* **4** 397. PMID: 12850190.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 75 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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