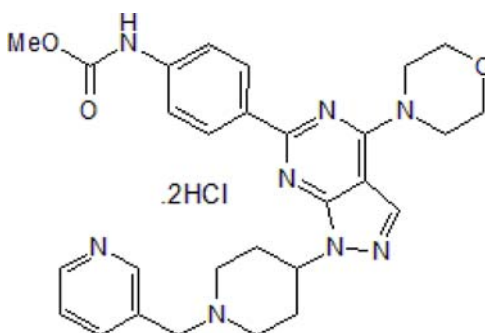


Product Name: WYE 687 **Catalog No.:** 4282 **Batch No.:** 1
CAS Number: 1702364-87-1
IUPAC Name: N-[4-[4-(4-Morpholinyl)-1-[1-(3-pyridinylmethyl)-4-piperidinyl]-1H-pyrazolo[3,4-d]pyrimidin-6-yl]phenyl]-carbamic acid methyl ester dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₂N₈O₃·2HCl·2H₂O
Batch Molecular Weight: 637.56
Physical Appearance: Pale brown solid
Solubility: water to 100 mM
DMSO to 100 mM
Storage: Desiccate at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Chloroform:Methanol:Ammonia soln. [95:5:0.1])
HPLC: Shows 98.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 52.75 | 6.01 | 17.58 |
| Found | 52.54 | 5.7 | 17.51 |

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

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Description:

Potent, ATP-competitive inhibitor of mammalian target of rapamycin (mTOR) (IC₅₀ = 7 nM). Displays selectivity for mTOR over PI 3-Kα (~100-fold) and PI 3-Kγ (~500-fold). Inhibits phosphorylation of mTORC1 and mTORC2 substrates including S6K, SGK and Akt; blocks VEGF secretion and HIF-1α expression. Exhibits antiproliferative effects in cancer cell lines through G₁ cell cycle arrest and selective apoptosis.

Physical and Chemical Properties:

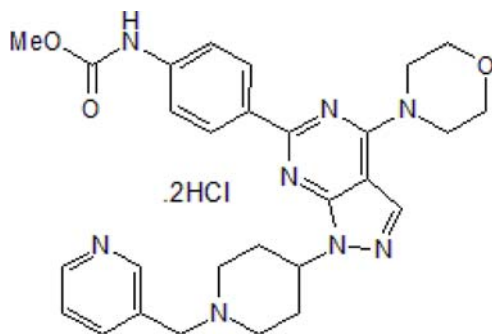
Batch Molecular Formula: C₂₈H₃₂N₈O₃.2HCl.2H₂O

Batch Molecular Weight: 637.56

Physical Appearance: Pale brown solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Yu *et al* (2009) Biochemical, cellular, and in vivo activity of novel ATP-competitive and selective inhibitors of the mammalian target of rapamycin. *Cancer.Res.* **69** (15) 6232. PMID: 19584280.

Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

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