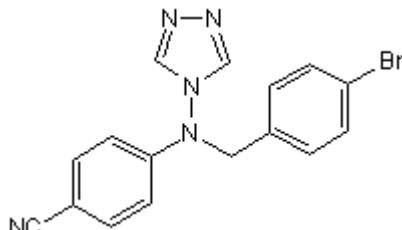


Certificate of Analysiswww.tocris.com**Product Name:** YM 511**Catalog No.:** 3278**Batch No.:** 1

CAS Number: 148869-05-0

IUPAC Name: 4-[(4-Bromophenyl)methyl]-4*H*-1,2,4-triazol-4-ylamino]benzonitrile**1. PHYSICAL AND CHEMICAL PROPERTIES****Batch Molecular Formula:** C₁₆H₁₂BrN₅**Batch Molecular Weight:** 354.2**Physical Appearance:** White solid**Solubility:** DMSO to 100 mM
ethanol to 25 mM**Storage:** Store at RT**Batch Molecular Structure:****2. ANALYTICAL DATA****TLC:** R_f = 0.69 (Dichloromethane:Methanol [9:1])**HPLC:** Shows 100% purity**¹H NMR:** Consistent with structure**Mass Spectrum:** Consistent with structure**Microanalysis:** Carbon Hydrogen Nitrogen

Theoretical 54.26 3.41 19.77

Found 54.07 3.46 19.75

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Product Information

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Product Name: YM 511

Catalog No.: 3278

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CAS Number: 148869-05-0

IUPAC Name: 4-[(4-Bromophenyl)methyl]-4*H*-1,2,4-triazol-4-ylamino]benzonitrile

Description:

Orally active, potent aromatase (CYP19) inhibitor (IC_{50} values are 0.4 and 0.12 nM at rat ovary and human placenta cells respectively) that only weakly inhibits the synthesis of other steroid hormones. Reduces plasma estrogen levels into ranges induced by ovariectomy and inhibits testosterone-induced breast cancer cell growth in vitro (IC_{50} = 0.13 nM).

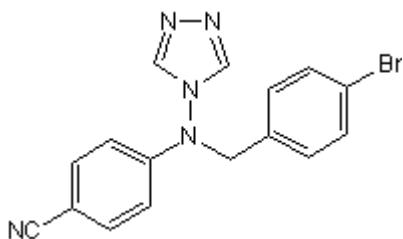
Physical and Chemical Properties:

 Batch Molecular Formula: $C_{16}H_{12}BrN_5$

Batch Molecular Weight: 354.2

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

 DMSO to 100 mM
 ethanol to 25 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:

Kudoh et al (1995) The potent and selective inhibitor of estrogen production by non-steroidal aromatase inhibitor, YM511. *J.Steroid Biochem.Molec.Biol.* **54** 265.

Kudoh et al (1996) Inhibitory effect of a novel non-steroidal aromatase inhibitor, YM511 on the proliferation of MCF-7 human breast cancer cell. *J.Steroid Biochem.Molec.Biol.* **58** 189.

Okada et al (1996) Studies on aromatase inhibitors I. Synthesis and biological evaluation of 4-amino-4*H*-1,2,4-triazole derivatives. *Chem.Pharm.Bull.* **44** 1871. PMID: 8904814.

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