

Certificate of Analysis

Product Name: YM 511

Catalog No.: 3278

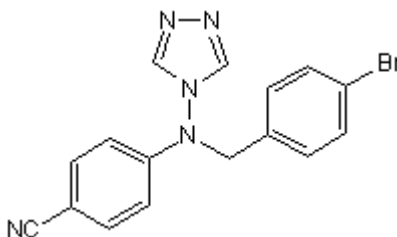
Batch No.: 1

CAS Number: 148869-05-0

IUPAC Name: 4-[[[(4-Bromophenyl)methyl]-4H-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

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

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Description:

Orally active, potent aromatase (CYP19) inhibitor (IC₅₀ 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 (IC₅₀ = 0.13 nM).

Physical and Chemical Properties:

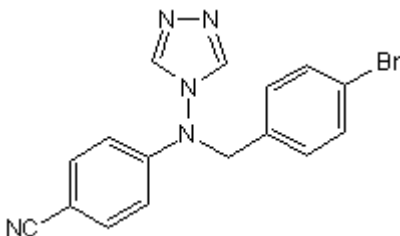
Batch Molecular Formula: C₁₆H₁₂BrN₅

Batch Molecular Weight: 354.2

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Kudoh et al (1995) The potent and selective inhibition 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-4H-1,2,4-triazole derivatives. *Chem. Pharm. Bull.* **44** 1871. PMID: 8904814.

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.

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