

**Product Name:** (Z)-4-Hydroxytamoxifen

**Catalog No.:** 3412

**Batch No.:** 10

**CAS Number:** 68047-06-3

**IUPAC Name:** 4-[(1Z)-1-[4-[2-(Dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phenol

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>26</sub>H<sub>29</sub>NO<sub>2</sub>·¼H<sub>2</sub>O

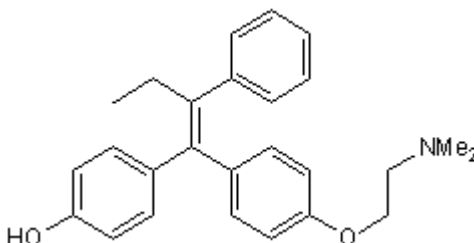
**Batch Molecular Weight:** 392.01

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.3 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	79.66	7.58	3.57
Found	79.58	7.59	3.55

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

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**Description:**

Estrogen receptor antagonist. Tamoxifen (Cat. No. 0999) metabolite; exhibits greater potency than the parent compound. Chemotherapeutic agent. Also activates intein-linked inactive Cas9, reducing off-target CRISPR-mediated gene editing; system has ~25-fold higher specificity than wtCas9.

**Physical and Chemical Properties:**

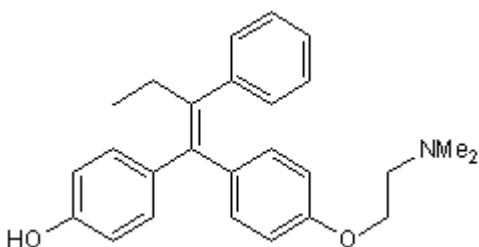
Batch Molecular Formula: C<sub>26</sub>H<sub>29</sub>NO<sub>2</sub> · ¼H<sub>2</sub>O

Batch Molecular Weight: 392.01

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 mM

CAUTION - This product has been shown\* to isomerise rapidly once in solution in most solvents, especially those with a low dielectric constant. Therefore, we recommend that, as far as possible, solutions should be made up and used immediately. The isomerisation process can be precluded by storage at -25°C in the dark as a solution in THF containing ca. 0.025% BHT.\*  
\*Katzenellenbogen *et al*/Synthesis of the (E) and (Z) isomers of the antiestrogen tamoxifen and its metabolite, hydroxytamoxifen, in tritium-labeled form (1982) J. Org. Chem. 47 2387.

**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:**

**Davis *et al*** (2015) Small molecule-triggered Cas9 protein with improved genome-editing specificity. *Nat.Chem.Biol.* **11** 316. PMID: 25848930.

**Desta *et al*** (2004) Comprehensive evaluation of tamoxifen sequential biotransformation by the human cytochrome P450 system in vitro: Prominent roles for CYP3A and CYP2D6. *J.Pharm.Exp.Ther.* **310** 1062. PMID: 15159443.

**Yu and Forman** (2003) Simple and efficient production of (Z)-4-hydroxytamoxifen, a potent estrogen receptor modulator. *J.Org.Chem.* **68** 9489. PMID: 14629178.

**Jordan *et al*** (1977) A monohydroxylated metabolite of tamoxifen with potent antioestrogenic activity. *J.Endocrinology* **75** 305. PMID: 591813.

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