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Certificate of Analysis

www.tocris.com

Catalog No.: 3412

Print Date: Feb 24th 2022

Batch No.: 12

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

CAS Number: 68047-06-3 IUPAC Name: 4-[(1*Z*)-1-[4-[

4-[(1Z)-1-[4-[2-(Dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₂₆H₂₉NO₂. 387.51 White solid DMSO to 100 mM ethanol to 20 mM Store at +4°C

Storage: **Batch Molecular Structure:**

NM e₂ HO

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 99.0% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen				
Theoretical	80.59	7.54	3.61		
Found	80.52	7.55	3.9		

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

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Product Information

Batch No.: 12

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Product Name: (Z)-4-Hydroxytamoxifen

CAS Number: 68047-06-3

4-[(1Z)-1-[4-[2-(Dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phenol

Description:

IUPAC Name:

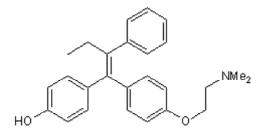
(Z)-4-Hydroxytamoxifen is an estrogen receptor antagonist (IC₅₀ = 27 μ M). (Z)-4-Hydroxytamoxifen is a Tamoxifen (Cat. No. 0999) metabolite; that exhibits greater potency than the parent compound. (Z)-4-Hydroxytamoxifen also activates intein-linked inactive Cas9, reducing off-target CRISPR-mediated gene editing; system has ~25-fold higher specificity than wtCas9. (Z) -4-Hydroxytamoxifen binds to voltage-gated sodium channels, near the intracellular gate and inhibits the sodium current by delaying channel recovery from the inactivated state (IC₅₀ values are 297 nM and 2.1 μ M for NavM and human Nav, respectively in HEK cells); this inhibitio... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₉NO₂. Batch Molecular Weight: 387.51 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.

Catalog No.: 3412

Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

Sula et al (2021) A tamoxifen receptor within a voltage-gated sodium channel. Mol.Cell. 81 1160. PMID: 33503406.

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 tamox. sequential biotransformation by the human cytochrome P450 system in vitro: Prominent roles for CYP3A and CYP2D6. J.Pharm.Exp.Ther. **310** 1062. PMID: 15159443.

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