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DATASHEET

4-Hydroxytamoxifen (E) and (Z) isomers (50:50)

Product overview

Name	4-Hydroxytamoxifen (E) and (Z) isomers (50:50)
Cat No	HB6095
Alternative names	4-OHT, Afimoxifene, H6278, 4-HT, 4-OH-TAM, OHT, TAM, 4-Hydroxytamoxifen, tamoxifen, z-4oht
Biological action	Activator
Purity	>98%
Description	Synthetic estrogen receptor ligand. Widely used in genome engineering (e.g. CreER/ CRISPR-Cas9).

Biological Data

Biological description Cell permeable, synthetic estrogen receptor ligand. Widely used in genome engineering. (E) and (Z) isomer mix (50:50).

CreER system:

De facto standard compound in drug-inducible manipulation of CreER recombinase. Allows external temporal control of Cre activity *in vivo*.

May also be used for TRAPing / in the TRAP / TRAP2 system (Targeted recombination in active populations).

CRISPR/Cas9 gene editing:

Activates an inactivated Cas9 nuclease (rendered inactive by insertion of a 4-OHT dependent-intein) to reduce off-target CRISPR-mediated gene editing (once bound with 4-OHT, conditionally active Cas9s modify target genomic sites with ~25-fold higher specificity than wild-type Cas9).

Also allows tight, repeated on-off control of the nuclease activity of the 'iCas' Cas9 variant which shows high editing efficiency at multiple loci once bound with 4-OHT.

Pure (Z)-4-hydroxytamoxifen also available.

≥70% Z isomer (remainder primarily E-isomer) 4-Hydroxytamoxifen also available.

Solubility & Handling

Storage instructions	-20°C
Solubility overview	Soluble in DMSO (100 mM) and in ethanol (50 mM)
Handling	<u>Storage of solid</u>

- This compound is light sensitive; exposure to light may affect compound performance. You should therefore store the material in the dark and protect from light.

Storage of solutions

- Do not store the material in solution; make up solutions and use immediately.
- The compound has been shown to isomerise rapidly in solution in most solvents (particularly solvents with a low dielectric constant). You should therefore make up and use solutions immediately.
- The isomerisation process can be precluded by storage of the compound at -25 °C in the dark as a THF solution containing ca. 0.025% BHT. (Katzenellenbogen et al (1982) J. Org. Chem. 47 2387.)

Important

This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use.

Chemical Data

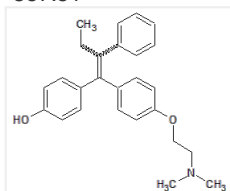
Chemical name

4-(1-[4-(Dimethylaminoethoxy)phenyl]-2-phenyl-1-butenyl)phenol

Molecular Weight

387.51

Chemical structure



Molecular Formula

C₂₆H₂₉NO₂

CAS Number

68392-35-8

PubChem identifier

449459

SMILES

CC/C(=C(\C1=CC=C(C=C1)O)/C2=CC=C(C=C2)OCCN(C)C)/C3=CC=CC=C3

Source

Synthetic

InChi

InChI=1S/C26H29NO2/c1-4-25(20-8-6-5-7-9-20)26(21-10-14-23(28)15-11-21)22-12-16-24(17-13-22)29-19-18-27(2)3/h5-17,28H,4,18-19H2,1-3H3/b26-25-

InChiKey

TXUZVZSFRXZGTL-QPLCGJKRSA-N

Appearance

Off-white solid

References

A monohydroxylated metabolite of tamoxifen with potent antioestrogenic activity.

Jordan et al (1977) J Endocrinol 75(2)

PubMedID

591813

A chemical-inducible CRISPR-Cas9 system for rapid control of genome editing.

Liu et al (2016) Nat Chem Biol 12(11)

PubMedID

27618190

Small molecule-triggered Cas9 protein with improved genome-editing specificity.

Small molecule-triggered Cas9 protein with improved genome-editing specificity. (2015) Nat Chem Biol 11(5)

PubMedID

25848930

Simple and efficient production of (Z)-4-hydroxytamoxifen, a potent estrogen receptor modulator.

Yu and Forman (2003) J Org Chem 68(24)

PubMedID

14629178