Nonsteroidal aromatase inhibitor 1

Cat. No.: HY-150775

CAS No.: 3033282-93-5

Molecular Formula: $C_{22}H_{16}N_4O_2$

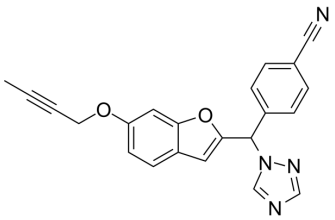
Molecular Weight: 368.39

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (271.45 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.7145 mL	13.5726 mL	27.1451 mL
5 mM	0.5429 mL	2.7145 mL	5.4290 mL
10 mM	0.2715 mL	1.3573 mL	2.7145 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.79 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.79 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Nonsteroidal aromatase inhibitor 1 (Compound 13h) is a nonsteroidal aromatase (CYP19A1) inhibitor (IC_{50}=0.09 nM). Nonsteroidal aromatase inhibitor 1 has potential for breast cancer research[1]. Nonsteroidal aromatase inhibitor 1 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

Aromatase

In Vitro

Nonsteroidal aromatase inhibitor 1 (0.001 pM-100 pM; 1 h) treatment shows excellent aromatase inhibition activity[1].
Nonsteroidal aromatase inhibitor 1 (1 μM; 48 h) treatment has no impact on MCF-10A or MDA-MB-231 growth[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	JEG-3 cells
Concentration:	0.001 pM-100 pM
Incubation Time:	1 hour
Result:	Showed excellent aromatase inhibition with the IC_{50} value of 0.09 nM.

Cell Cytotoxicity Assay[1]

Cell Line:	MCF-10A and MDA-MB-231 cells
Concentration:	1 μM
Incubation Time:	48 hour
Result:	Suggested possible limited toxicity in normal breast tissue and little off-target effects.

REFERENCES

[1]. Ahmed G Eissa, et al. 4th generation nonsteroidal aromatase inhibitors: An iterative SAR-guided design, synthesis, and biological evaluation towards picomolar dual binding inhibitors. Eur J Med Chem. 2022 Jul 6;240:114569.

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