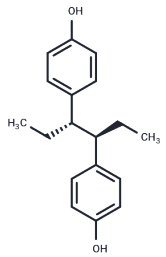
Data Sheet (Cat.No.T6533)

TargetMol

Hexestrol

Chemical Properties



CAS No. : 84-16-2

Formula: C18H22O2

Molecular Weight: 270.37

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Hexestrol (Hexanoestrol) binds to ERα and ERβ with EC50 of 0.07 nM and 0.175 nM, respectively.
Targets(IC50)	Estrogen Receptor/ERR,Estrogen/progestogen Receptor
In vitro	Hexestrol binds to ERα with EC50 of 0.07 nM and to ERβ with EC50 of 0.175 nM. [1] Hexestrol inhibits activity of AKR1B13 with IC50 of 3.2 μM. [2] Hexestrol inhibits the d-galactose dehydrogenase activity of thermophilus aldose 1-dehydrogenase with IC50 of 0.063 mM. [3] Hexestrol inhibits the dehydrogenase activity of AKR1C20 towards 10 μM 4-androsten-3α-o1-17-one with IC50 values of 2.7 μM. [4] Hexestrol inhibits 17HSD5 with IC50 of 30 μM, and inhibits TBER1 with IC50 of 0.8 μM. [5] Hexestrol reacts with DNA through the catechol quinone, thus can be a carcinogen. [6]
In vivo	Hexestrol administered intraperitoneally at dose of 6 mg/kg may decrease ovulation in mice, as evident by smaller ovaries and decreased luteal bodies and oocytes. [7]

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble or slightly soluble), DMSO: 55 mg/mL (203.42 mM),Sonication is recommended. Ethanol: 39 mg/mL (144.25 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 5.5 mg/mL (20.34 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5.5 mg/mL (20.34 mM),Solution. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.6986 mL	18.4932 mL	36.9864 mL
5 mM	0.7397 mL	3.6986 mL	7.3973 mL
10 mM	0.3699 mL	1.8493 mL	3.6986 mL
50 mM	0.074 mL	0.3699 mL	0.7397 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Waibel M, et al. Eur J Med Chem, 2009, 44(9), 3412-3424.
Endo S, et al. Chem Biol Interact, 2009, 178(1-3), 151-157.
Asada Y, et al. Chem Biol Interact. 2009, 178(1-3), 117-126.
Matsumoto K, et al. Biol Pharm Bull, 2006, 29(3), 539-542.
Ishikura S, et al. J Biochem, 2006, 139(6), 1053-1063.