Pregnenolone 16α-carbonitrile

Cat. No.: HY-131723

CAS No.: 1434-54-4

Molecular Formula: $C_{22}H_{31}NO_2$

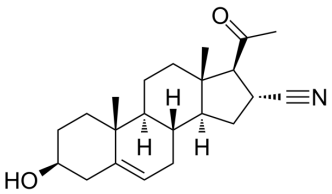
Molecular Weight: 341.49

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage:

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : 20 mg/mL (58.57 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9283 mL	14.6417 mL	29.2834 mL
	5 mM	0.5857 mL	2.9283 mL	5.8567 mL
	10 mM	0.2928 mL	1.4642 mL	2.9283 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.43 mg/mL (4.19 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.43 mg/mL (4.19 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Pregnenolone 16α-carbonitrile is an orally active prototypical and effective rodent-PXR activator. Pregnenolone 16α-carbonitrile, a synthetic steroid, induces cytochrome P450 3A expression. Pregnenolone 16α-carbonitrile exhibits increased resistance to subsequent stressful insults[1][2][3].

In Vitro

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

In Vivo

Pregnenolone 16α-carbonitrile (40 mg/kg/day; i.p.; for two days) induces the expression of Cyp3a11 and Cyp2b10 at the mRNA, protein, and enzymatic levels in WT mice[1].

Pregnenolone 16α-carbonitrile (100 mg/kg; ip; single dose) induces the expression of CYP3A mRNA in adult female Sprague-Dawley rats weighing 150-200 g[2].

Pregnenolone 16α-carbonitrile (35 mg/kg; gavage; once daily for three days) increase in Pgp expression in male Sprague-Dawley rats, aged approximately 100 days and weighing 250-400 g[3].

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

Animal Model:	WT and $Pxr^{-/-}$ mice[1]
Dosage:	40 mg/kg
Administration:	IP; per day for two days
Result:	Induced the expression of Cyp3a11 and Cyp2b10 at the mRNA, protein, and enzymatic levels in WT mice. Had little effect on the expression of Cyp3a11 in $Pxr^{-/-}$ mice

CUSTOMER VALIDATION

- bioRxiv. 2023 Feb 4.

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REFERENCES

[1]. Yang Xie, et al. Activation of Pregnane X Receptor Sensitizes Mice to Hemorrhagic Shock-Induced Liver Injury. Hepatology. 2019 Sep;70(3):995-1010.

[2]. Simon Lowes, et al. The Effects of Pregnenolone 16α-Carbonitrile Dosing on Digoxin Pharmacokinetics and Intestinal Absorption in the Rat. Pharmaceutics. 2010 Mar 15;2(1):61-77.

[3]. Jeffrey Guzelian, et al. Identification of genes controlled by the pregnane X receptor by microarray analysis of mRNAs from pregnenolone 16alpha-carbonitrile-treated rats. Toxicol Sci. 2006 Dec;94(2):379-87.

[4]. Carylyn J Marek, et al. Pregnenolone-16alpha-carbonitrile inhibits rodent liver fibrogenesis via PXR (pregnane X receptor)-dependent and PXR-independent mechanisms. Biochem J. 2005 May 1;387(Pt 3):601-8.

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