Product Data Sheet

Product Name: Pregnenolone Carbonitrile
Cat. No.: GC17893

Chemical Properties

Cas. No.	1434-54-4		
Chemical Name	3β-hydroxy-20-oxo-pregn-5-ene-16α-carbonitrile		
SMILES	O[C@H](C1)CC[C@@]2(C)C1=CC[C@]3([H])[C@]2([H])CC[C@@]4(C)[C@@]3([H])C[C@@H](C#N)[C@@H]4C(C)=O		
Formula	$C_{22}H_{31}NO_2$	M.Wt	341.5
Solubility	≤1mg/ml in ethanol;1mg/ml in methanol;1mg/ml in acetonitrile; 10mg/mL in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Pregnenolone Carbonitrile		

Background

Pregnenolone-16α-carbonitrile is a rodent pregnane X receptor (PXR) activator involved in inducing the synthesis of a unique cytochrome P450 peptide in hepatic microsomes of male rats [1].

The nuclear pregnane X receptor (PXR) is an important component of the body’s adaptive defense mechanism against toxic substances. PXR could be activated by a large number of endogenous and exogenous chemicals such as antibiotics, steroids, antimycotics, and bile acids. PXR acts as a generalized sensor of hydrophobic toxins. PXR heterodimer binds with the 9-cis retinoic acid receptor (NR2B) to DNA response elements in the regulatory regions of cytochrome P450 3A monooxygenase genes and a number of other genes involved in the metabolism and elimination of xenobiotics from

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the body [2].

In vitro: In rat HSCs, PCN inhibited the trans-differentiation of rat HSCs in vitro despite the absence of PXR expression [3].

In vivo: PCN administration (25 mg/kg; one injection/week) to rats significantly increased the relative liver weight. In rats, PCN administration did not result in liver damage or significantly affect the level of liver damage caused by carbon tetrachloride. PCN treatment to carbon tetrachloride-treated rats resulted in a significant decrease in both intralobular α-smooth-muscle-actin immunostaining and intense Sirius Red staining in liver sections. PCN didn’t interfere with the metabolism of carbon tetrachloride to toxic metabolites [3].

□□-16α-□□□□□□□□□X□□□PXR□□□□□□□□□□□□□□□□□□□□□□□□□□P450□□□□[1]□

□□□X□□□PXR□□□□□□□□□□□□□□□□□□□□□□□□PXR□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□PXR□□□□□□□□□□□□□□PXR□□□□□9-□□□□□□□□NR2B□□□□□□□□P450 3A□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□DNA□□□□[2]□

□□□□□□HSCs□□□□□□PXR□□□PCN□□□□□□HSCs□□□□[3]□

□□□□PCN□□□25 mg/kg□□□□□□□□□□□□□□□□□□□□□□□□□□□PCN□□PCN□□□□□□□□□□□□α-□□□□□□□□□□□□Sirius Red□□□□□□□PCN□□□□□□□□□□□□□□□□□□□[3]□

References:

[1] Birnbaum L S, Baird M B, Massie H R. Pregnenolone-16alpha-carbonitrile-inducible cytochrome P450 in rat liver[J]. Research communications in chemical pathology and pharmacology, 1976, 15(3): 553.
[2] Kliewer S A, Goodwin B, Willson T M. The nuclear pregnane X receptor: a key regulator of xenobiotic metabolism[J]. Endocrine reviews, 2002, 23(5): 687-702.
[3] Marek C J, Tucker S J, Konstantinou D K, et al. Pregnenolone-16α-carbonitrile inhibits rodent liver fibrogenesis via PXR (pregnane X receptor)-dependent and PXR-independent mechanisms[J]. Biochemical Journal, 2005, 387(3): 601-608.

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