

Product Name: 20(S)-Hydroxycholesterol

Catalog No.: 4474

Batch No.: 3

CAS Number: 516-72-3

IUPAC Name: (3 β)-Cholest-5-ene-3,20-diol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₄₆O₂· $\frac{1}{4}$ H₂O

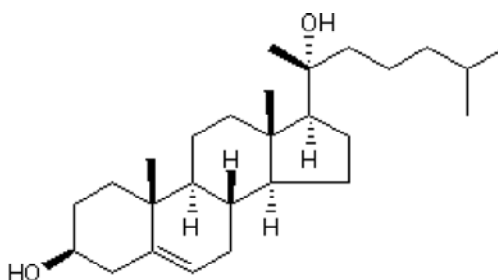
Batch Molecular Weight: 407.15

Physical Appearance: White solid

Solubility: ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.36 (Ethyl acetate:Petroleum ether [3:7])

Melting Point: Between 135 - 136°C

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -65.3 (Concentration = 0.23, Solvent = Chloroform)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 79.65 11.51

Found 79.64 11.56

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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CAS Number: 516-72-3

IUPAC Name: (3 β)-Cholest-5-ene-3,20-diol

Description:

20(S)-Hydroxycholesterol is an allosteric activator of the Hedgehog signaling pathway Smoothed (Smo) oncoprotein; binds at a site distinct from the canonical cyclopamine binding site. Activates Hedgehog (Hh) signaling ($EC_{50} \sim 3\mu\text{M}$ for induction of Hh reporter gene transcription in NIH 3T3 cells). Induces Smo accumulation in primary cilia; also exhibits osteogenic activity and activates the liver X receptor (LXR).

Physical and Chemical Properties:

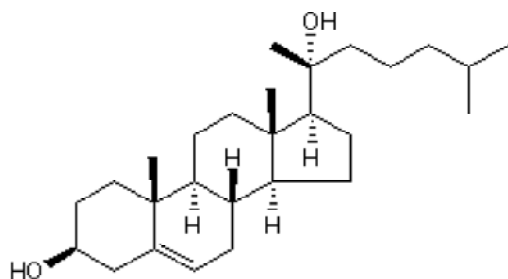
Batch Molecular Formula: $C_{27}H_{46}O_2 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 407.15

Physical Appearance: White solid

Minimum Purity: $\geq 95\%$

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}\text{C}$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Nedelcu *et al* (2013) Oxysterol binding to the extracellular domain of Smoothed in Hedgehog signaling. *Nat.Chem.Biol.* **9** 557. PMID: 23831757.

Nachtergaele *et al* (2012) Oxysterols are allosteric activators of the oncoprotein Smoothed. *Nat.Chem.Biol.* **8** 211. PMID: 22231273.

Dwyer *et al* (2007) Oxysterols are novel activators of the hedgehog signaling pathway in pluripotent mesenchymal cells *J.Biol.Chem.* **282** 8959. PMID: 17200122.

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