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PRODUCT INFORMATION

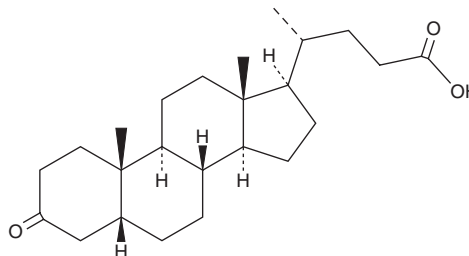


Dehydrolithocholic Acid

Item No. 29544

CAS Registry No.: 1553-56-6
Formal Name: (5 β)-3-oxo-cholan-24-oic acid
Synonyms: 3-keto LCA, 3-keto Lithocholate, 3-keto Lithocholic Acid, 3-KLCA, 3-oxo LCA, 3-oxo Lithocholate, 3-oxo Lithocholic Acid

MF: C₂₄H₃₈O₃
FW: 374.6
Purity: \geq 95%
Supplied as: A crystalline solid
Storage: -20°C
Stability: \geq 2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Dehydrolithocholic acid is supplied as a crystalline solid. A stock solution may be made by dissolving the dehydrolithocholic acid in the solvent of choice, which should be purged with an inert gas. Dehydrolithocholic acid is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of dehydrolithocholic acid in these solvents is approximately 10, 15, and 30 mg/ml, respectively.

Dehydrolithocholic acid is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, dehydrolithocholic acid should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Dehydrolithocholic acid has a solubility of approximately 0.20 mg/ml in a 1:4 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Dehydrolithocholic acid is a major metabolite of lithocholic acid (LCA; Item No. 20253).¹ It is formed from LCA by the cytochrome P450 (CYP) isoform CYP3A4. Dehydrolithocholic acid is an agonist of G protein-coupled bile acid activated receptor 1 (GP-BAR1/TGR5; EC₅₀ = 0.27 μ M), vitamin D receptor (VDR; EC₅₀ = 3 μ M), and farnesoid X receptor (FXR) in cell-based reporter assays.^{2,3} It also binds to the human pregnane X receptor (PXR; IC₅₀ = 15 μ M) and activates mouse and human PXR in cell-based reporter assays when used at a concentration of 100 μ M.⁴ Dehydrolithocholic acid binds to retinoic acid receptor-related orphan receptor γ t (ROR γ t; K_d = 1.13 μ M for the recombinant human ligand-binding domain) and decreases its activity in a cell-based reporter assay when used at a concentration of 10 μ M.⁵ It inhibits the differentiation of T helper cells that express IL-17a (T_H17 cells) when used at a concentration of 20 μ M.

References

1. Deo, A.K. and Bandiera, S.M. 3-Ketocholanoic acid is the major in vitro human hepatic microsomal metabolite of lithocholic acid. *Drug Metab. Dispos.* **37**(9), 1938-1947 (2009).
2. Sato, H., Macchiarulo, A., Thomas, C., et al. Novel potent and selective bile acid derivatives as TGR5 agonists: Biological screening, structure-activity relationships, and molecular modeling studies. *J. Med. Chem.* **51**(6), 1831-1841 (2008).
3. Makishima, M., Lu, T.T., Xie, W., et al. Vitamin D receptor as an intestinal bile acid sensor. *Science* **296**(5571), 1313-1316 (2002).
4. Staudinger, J.L., Goodwin, B., Jones, S.A., et al. The nuclear receptor PXR is a lithocholic acid sensor that protects against liver toxicity. *Proc. Natl. Acad. Sci. USA* **98**(6), 3369-3374 (2000).
5. Hang, S., Paik, D., Yao, L., et al. Bile acid metabolites control T_H17 and T_{reg} cell differentiation. *Nature* **576**(7785), 143-148 (2019).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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