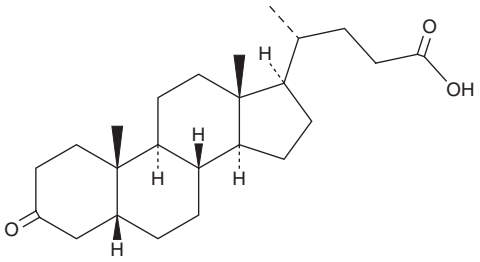
PRODUCT INFORMATION

Dehydrolithocholic Acid

Item No. 29544

CAS Registry No.:	1553-56-6
Formal Name:	(5β)-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:	$C_{24}H_{38}O_3$
FW:	374.6
Purity:	≥95%
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 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; EC_{50} = 0.27 µM), vitamin D receptor (VDR; EC_{50} = 3 µM), and farnesoid X receptor (FXR) in cell-based reporter assays.[2,3] It also binds to the human pregnane X receptor (PXR; IC_{50} = 15 µM) and activates mouse and human PXRs in cell-based reporter assays when used at a concentration of 100 µM.[4] Dehydrolithocholic acid binds to retinoic acid receptor-related orphan receptor γt (RORγt; K_d = 1.13 µM for the recombinant human ligand-binding domain) and decreases its activity in a cell-based reporter assay when used at a concentration of 10 µM.[5] It inhibits the differentiation of T helper cells that express IL-17a (T_H17 cells) when used at a concentration of 20 µM.

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).

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