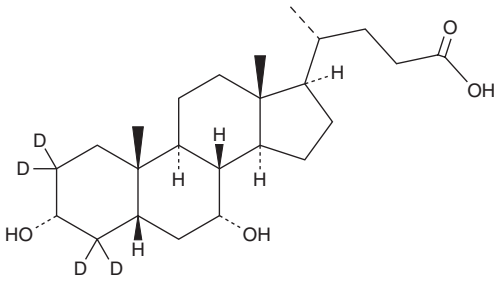
PRODUCT INFORMATION

Chenodeoxycholic Acid-d_4

Item No. 20848

CAS Registry No.: 99102-69-9
Formal Name: 3α,7α-dihydroxy-5β-cholan-24-oic-2,2,4,4-d4 acid
Synonym: CDCA-d_4
MF: $C_{24}H_{36}D_4O_4$
FW: 396.6
Chemical Purity: ≥95% (Chenodeoxycholic Acid)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_4); ≤1% d_0
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



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

Laboratory Procedures

Chenodeoxycholic acid-d_4 (CDCA-d_4) is intended for use as an internal standard for the quantification of CDCA (Item No. 10011286) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

CDCA-d_4 is supplied as a crystalline solid. A stock solution may be made by dissolving the CDCA-d_4 in the solvent of choice. CDCA-d_4 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of CDCA-d_4 in DMF is approximately 30 mg/ml and approximately 20 mg/ml in ethanol and DMSO.

CDCA-d_4 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CDCA-d_4 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. CDCA-d_4 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

CDCA is a hydrophobic primary bile acid.[1] It is formed from cholesterol in the liver *via* a multistep process catalyzed by the cytochrome P450 (CYP) isoforms CYP7A1, CYP8B1, and CYP27A1. CDCA is a farnesoid X receptor (FXR) agonist that binds to FXRs in a TR-FRET assay (EC_{50} = 13 µM) and induces FXR transactivation in a reporter assay.[2,3] It induces transcription of the gene encoding the Nrf2 target glutamate cysteine ligase (GCL) in primary hepatocytes and HepG2 cells when used at concentrations ranging from 25 to 100 µM.[4]

References

1. Fiorucci, S. and Distrutti, E. Chenodeoxycholic acid: An update on its therapeutic applications. *Bile acids and their receptors. Handbook of experimental pharmacology*. Fiorucci, S. and Distrutti, E., 1st edition, *Springer* (2019).
2. Ohinata, Y., Payer, B., O'Carroll, D., *et al*. *Nature* **436**, 207-213 (2005).
3. Urizar, N.L., Liverman, A.B., Dodds, D.T., *et al*. *Science* **296(5573)**, 1703-1706 (2002).
4. Tan, K.P., Yang, M., and Ito, S. *Mol. Pharmacol*. **72(5)**, 1380-1390 (2007).

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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