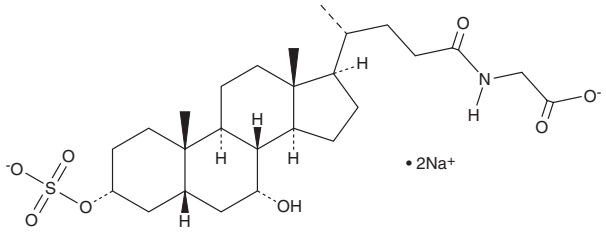
PRODUCT INFORMATION

Glycochenodeoxycholic Acid 3-sulfate (sodium salt)

Item No. 45839

CAS Registry No.: 66874-09-7
Formal Name: N-[(3α,5β,7α)-7-hydroxy-24-oxo-3-(sulfooxy) cholan-24-yl]-glycine, disodium salt
Synonyms: GCDCA-S, Glycochenodeoxycholic Acid 3-O-sulfate
MF: $C_{26}H_{41}NO_8S \bullet 2Na$
FW: 573.7
Purity: ≥98%
Supplied as: A 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

Glycochenodeoxycholic acid 3-sulfate (GCDCA-S) (sodium salt) is supplied as a solid. A stock solution may be made by dissolving the GCDCA-S (sodium salt) in the solvent of choice, which should be purged with an inert gas. GCDCA-S (sodium salt) is sparingly soluble (1-10 mg/ml) in DMSO and slightly soluble (0.1-1 mg/ml) in methanol.

GCDCA-S (sodium salt) is slightly soluble in aqueous solutions. To enhance aqueous solubility, dilute the organic solvent solution into aqueous buffers or isotonic saline. If performing biological experiments, ensure the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. We do not recommend storing the aqueous solution for more than one day.

Description

GCDCA-S is a metabolite of glycochenodeoxycholic acid (Item Nos. 16942 | 44904), the glycine-conjugated form of the primary bile acid chenodeoxycholic acid (Item Nos. 10011286 | 35346 | 44867).[1,2] It is formed from glycochenodeoxycholic acid by sulfonation *via* sulfotransferase 2A1 (SULT2A1). GCDCA-S is a substrate of organic anion transporting polypeptide 1B1 (OATP1B1), OATP1B3 and organic anion transporter (OAT3), and GCDCA-S uptake is inhibited by the OATP1B1/3 inhibitor rifampicin (Item No. 14423) in primary human hepatocytes.[3]

References

1. Alnouti, Y. Bile acid sulfation: A pathway of bile acid elimination and detoxification. *Toxicol. Sci.* **108(2),** 225-246 (2009).
2. Ujihira, Y., Georgiev, V., Ogungbenro, K., *et al.* Population pharmacokinetic modeling of glycochenodeoxycholic acid 3-O-sulfate (GCDCA-S) as endogenous biomarker of OATP1B3 and OAT3 transporters. *Clin. Pharmacol. Ther.* **118(6),** 1532-1542 (2025).
3. Orozco, C.C., Neuvonen, M., Bi, Y.-A., *et al.* Characterization of bile acid sulfate conjugates as substrates of human organic anion transporting polypeptides. *Mol. Pharm.* **20(6),** 3020-3032 (2023).

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.

WARRANTY AND LIMITATION OF REMEDY
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CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM