CHENODEOXYCHOLIC ACID

Conjugated Pooled Standards





Redefine host-microbiome relationships with 22 unique microbially-derived bile acid compounds

Gut microbes convert liver-produced bile acids into secondary bile acids with diverse chemistry and biological impact on humans and animals. Hundreds of these compounds were recently discovered in mammals with yet-to-be-discovered biological functions and health impacts^{1,2}.

Amide conjugations to chenodeoxycholic acid and other bile acids represent a novel class of next-generation biomarkers with the potential to revolutionize the treatment and diagnostics of gut microbiome-related diseases, including inflammatory bowel disease and cystic fibrosis3. You can now participate in this exciting research and development field using these pooled standards of chenodeoxycholic acid amidates (amine conjugates to the carboxylic acid of chenodeoxycholic acid) and your expertise in liquid chromatography (LC) and mass spectrometry (MS).

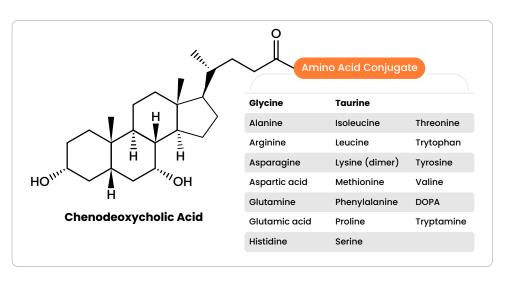
¹Quinn, Melnik, et al. (2020) *Nature*.

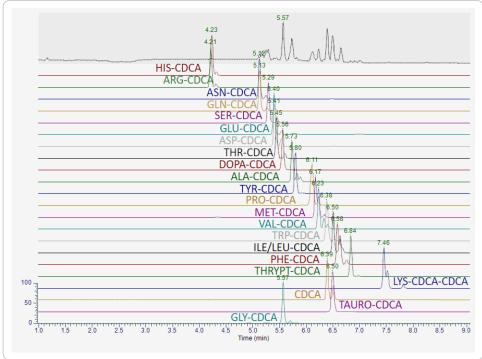
Global chemical effects of the microbiome include new bile-acid

conjugations

²Dorrestein, Melnik, Aksenov, Quinn. <u>US</u> Patent Application (#20220202881) for Bile Acids and Use in Disease Treatment

³Gentry, Collins, et al. (2023) *Nature*. Reverse metabolomics for the discovery of chemical structures from humans.





Reverse phase chromatogram of chenodeoxycholic acid amidates mixture







Product Characteristics:

| Compounds | 22 microbial cholic amidates plus unconjugated chenodeoxycholic acid | |
|--------------------------|--|--|
| Applications | Biomarker discovery | Bile acid metabolism |
| | Host-microbe interactions | Bile salt hydrolase/N-Acyl transferase |
| | Microbiome analysis & profiling | activity assessments |
| Contents | 5 mg dry powder (lyophilized) | |
| | Aliquoted into glass vials | |
| Analytical Examples | Compound identification | In-house digital library |
| | MS2 transitions | Method development |
| | Retention time acquisition | Biomarker quantification |
| Suitable for | HPLC | |
| | UHPLC | |
| MS compatibility | QTOF | Single quadrupole |
| | Orbitrap | Triple quadrupole |
| Concentration* | ■ 200 µg/mL | |
| Internal standard | Chenodeoxycholic acid (unconjugated) | |
| | • Quantity provided: | |
| | Glycochenodeoxycholic acid (GLY-CDCA) | |
| | Taurochenodeoxycholic acid (TAURO-CDCA) | |
| Certificate of Analysis^ | Reference retention times | |
| | Mass spectra | |

^ acquired under standard HPLC-MS conditions

Common Analytical Applications:

*Estimated from glycine and taurine conjugates

- Build an in-house library of retention times and mass spectra for compound identification
- Acquire and optimize MS/MS transitions for quantitative analysis
- Calibrate retention times of conjugated bile acids after changing LC method or column

Laboratory Chemical Safety Summary Datasheet Links #:

Taurochenodeoxycholic Acid

Glycochenodeoxycholic Acid

*No chemical safety information is currently available for all other novel amidates





