LITHOCHOLIC ACID

Conjugated **Pooled Standards**





Redefine host-microbiome relationships with 21 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 lithocholic 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 lithocholic acid amidates (amine conjugates to the carboxylic acid of lithocholic acid) and your expertise in liquid chromatography (LC) and mass spectrometry (MS).

Amino Acid Conjugate **Glycine** Taurine Serine Alanine Histidine Threonine Arginine Isoleucine Trytophan H **Asparagine** Leucine **Tyrosine** HO''' Aspartic acid Methionine Valine Glutamine Phenylalanine **Tryptamine Lithocholic Acid** Glutamic acid **Proline** GABA

HIS-LCA ARG-LCA GLN-LCA ASP-LCA SER-LCA **GLU-LCA** THR-LCA GABA-LCA TYR-LCA ALA-LCA PRO-I CA MET-LCA TRP-LCA ILE/LEU-LCA PHE-LCA THRYPT-LCA **GLY-LCA** TAURO-LCA LCA Time (min)

Reverse phase chromatogram of lithocholic acid amidates mixture

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.







Product Characteristics:

Compounds	 21 microbial cholic amidates plus unconjugated lithocholic 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	Lithocholic acid (unconjugated)	
	• Quantity provided:	
	Glycolithocholic acid (GLY-LCA)	
	Taurolithocholic acid (TAURO-LCA)	
Certificate of Analysis^	 Reference retention times 	
	Mass spectra	

^{*}Estimated from glycine and taurine conjugates

Common Analytical Applications:

- 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 #:

Taurolithocholic Acid

Glycolithocholic Acid

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







[^] acquired under standard HPLC-MS conditions