# **CHOLIC 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<sup>1,2</sup>.

Amide conjugations to cholic 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 cholic acid amidates (amine conjugates to the carboxylic acid of cholic acid) and your expertise in liquid chromatography (LC) and mass spectrometry (MS).

Amino Acid Conjugate Glycine Taurine Alanine Isoleucine Threonine Arginine Leucine Trytophan H Asparagine Lysine (dimer) Tyrosine HO'''  $^{\prime\prime}$ OH Aspartic acid Methionine Valine Glutamine Phenylalanine DOPA **Cholic Acid** Glutamic acid Proline **Tryptamine** Histidine Serine

ARG-CA ASN-CA SER-CA THR-CA DOPA-CA ALA-CA TYR-CA MET-CA ILE/LEU-CA PHE-CA TRYPT-CA LYS-CA-CA 100 50 TAURO-CA

Reverse phase chromatogram of cholic acid amidates mixture

<sup>1</sup>Quinn, Melnik, et al. (2020) *Nature*. Global chemical effects of the microbiome include new bile-acid conjugations

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

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







#### **Product Characteristics:**

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

^ 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 #:

**Taurocholic Acid** 

**Glycocholic Acid** 

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





