

**Supplemental Table S1 (Appendix)**

Abbreviations and corresponding trivial names of the Fatty acid-bile acid esters, fatty acids, and bile acids used in this study.

Abbreviations	Trivial names	Structure Lipid Maps ID
Fatty acid-bile acid ester		
Ac-isoLCA	3 $\beta$ -acetoxy-5 $\beta$ -cholanoic acid	
Pam-isoLCA	3 $\beta$ -hexadecanoyloxy-5 $\beta$ -cholanoic acid	
Ste-isoLCA	3 $\beta$ -octadecanoyloxy-5 $\beta$ -cholanoic acid	
Ole-isoLCA	3 $\beta$ -(9-cis-octadecenoyloxy)-5 $\beta$ -cholanoic acid	
Lin-isoLCA	3 $\beta$ -(9-cis,12-cis-octadecadienoyloxy)-5 $\beta$ -cholanoic acid	
Ac-isoDCA	3 $\beta$ -acetoxy-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Pam-isoDCA	3 $\beta$ -hexadecanoyloxy-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Ste-isoDCA	3 $\beta$ -octadecanoyloxy-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Ole-isoDCA	3 $\beta$ -(9-cis-octadecenoyloxy)-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Lin-isoDCA	3 $\beta$ -(9-cis,12-cis-octadecadienoyloxy)-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Ac-LCA	3 $\alpha$ -acetoxy-5 $\beta$ -cholanoic acid	
Ste-LCA	3 $\alpha$ -octadecanoyloxy-5 $\beta$ -cholanoic acid	
Ste-DCA	3 $\alpha$ -octadecanoyloxy-12 $\alpha$ -hydroxy-5 $\beta$ -cholanoic acid	
Fatty acid		
Palmitic acid	hexadecanoic acid	<a href="#">LMFA01010001</a>
Stearic acid	octadecanoic acid	<a href="#">LMFA01010018</a>
Oleic acid	9-cis-Octadecenoic acid	<a href="#">LMFA01030002</a>
Linoleic acid	9-cis,12-cis-Octadecadienoic acid	<a href="#">LMFA01030120</a>
Bile acid		
CA	cholic acid	<a href="#">LMST04010001</a>
alloCA	3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010092</a>
isoCA	3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010086</a>
3-oxo-CA	7 $\alpha$ ,12 $\alpha$ -dihydroxy-3-oxo-5 $\beta$ -cholanolic acid	<a href="#">LMST04010443</a>
7-oxo-DCA	3 $\alpha$ ,12 $\alpha$ -dihydroxy-7-oxo-5 $\beta$ -cholanoic acid	<a href="#">LMST04010184</a>
12-oxo-CDCA	3 $\alpha$ ,7 $\alpha$ -dihydroxy-12-oxo-5 $\beta$ -cholanolic acid	<a href="#">LMST04010180</a>
UCA	3 $\alpha$ ,7 $\beta$ ,12 $\alpha$ -trihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010088</a>
isoUCA	3 $\beta$ ,7 $\beta$ ,12 $\alpha$ -trihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010090</a>
HCA	3 $\alpha$ ,6 $\alpha$ ,7 $\alpha$ -trihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010064</a>
CDCA	chenodeoxycholic acid	<a href="#">LMST04010032</a>
alloCDCA	3 $\alpha$ ,7 $\alpha$ -dihydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010036</a>
isoCDCA	3 $\beta$ ,7 $\alpha$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010034</a>

3-oxo-CDCA	7 $\alpha$ -hydroxy-3-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010161</a>
3-oxo-alloCDCA	7 $\alpha$ -hydroxy-3-oxo-5 $\alpha$ -cholanic acid	<a href="#">LMST04010163</a>
7-oxo-LCA	3 $\alpha$ -hydroxy-7-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010150</a>
UDCA	Ursodeoxycholic acid	<a href="#">LMST04010033</a>
isoUDCA	3 $\alpha$ ,7 $\beta$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010035</a>
3-oxo-UDCA	7 $\beta$ -hydroxy-3-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010162</a>
DCA	deoxycholic acid	<a href="#">LMST04010040</a>
alloDCA	3 $\alpha$ ,12 $\alpha$ -dihydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010044</a>
isoDCA	3 $\beta$ ,12 $\alpha$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010042</a>
isoalloDCA	3 $\beta$ ,12 $\alpha$ -dihydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010046</a>
3-oxo-DCA	12 $\alpha$ -hydroxy-3-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010168</a>
3-oxo-alloDCA	12 $\alpha$ -hydroxy-3-oxo-5 $\alpha$ -cholanic acid	<a href="#">LMST04010169</a>
12 $\beta$ -OH-LCA	3 $\alpha$ ,12 $\beta$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010045</a>
12 $\beta$ -OH-isoLCA	3 $\beta$ ,12 $\beta$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010047</a>
12-oxo-LCA	3 $\alpha$ -hydroxy-12-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010155</a>
12-oxo-isoLCA	3 $\beta$ -hydroxy-12-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010156</a>
LCA	lithocholic acid	<a href="#">LMST04010003</a>
alloLCA	3 $\alpha$ -hydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010005</a>
isoLCA	3 $\beta$ -hydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010004</a>
isoalloLCA	3 $\beta$ -hydroxy-5 $\alpha$ -cholanoic acid	<a href="#">LMST04010006</a>
3-oxo-LCA	3-oxo-5 $\beta$ -cholanic acid	<a href="#">LMST04010127</a>
3-oxo-alloLCA	3-oxo-5 $\alpha$ -cholanic acid	<a href="#">LMST04010128</a>
HDCA	3 $\alpha$ ,6 $\alpha$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010024</a>
MDCA	3 $\alpha$ ,6 $\beta$ -dihydroxy-5 $\beta$ -cholanoic acid	<a href="#">LMST04010025</a>
CA- $\Delta^4$ -3-one	7 $\alpha$ ,12 $\alpha$ -dihydroxy-3-oxo-4-cholenoic acid	<a href="#">LMST04030114</a>
DCA- $\Delta^{4,6}$ -3-one	12 $\alpha$ -hydroxy-3-oxo-4,6-choladienoic acid	<a href="#">LMST04010245</a>
CDCA- $\Delta^4$ -3-one	7 $\alpha$ -hydroxy-3-oxo-4-cholenoic acid	<a href="#">LMST04030123</a>
LCA- $\Delta^{4,6}$ -3-one	3-oxo-4,6-choladienoic acid	<a href="#">LMST04010235</a>
DCA- $\Delta^4$ -3-one	12 $\alpha$ -hydroxy-3-oxo-4-cholenoic acid	<a href="#">LMST04010198</a>
LCA- $\Delta^4$ -3-one	3-oxo-4-cholenoic acid	<a href="#">LMST04010233</a>
nor-CA	3,7,12-trihydroxy-24-nor-5 $\beta$ -cholan-23-oic acid	<a href="#">LMST04060019</a>
GCA	glycocholic acid	<a href="#">LMST05030001</a>
TCA	taurocholic acid	<a href="#">LMST05040001</a>
CA-3S	cholic acid 3-sulfate	
GCA-3S	glycocholic acid 3-sulfate	
TCA-3S	taurocholic acid 3-sulfate	<a href="#">LMST05020031</a>
GCDCA	glycochenodeoxycholic acid	<a href="#">LMST05030008</a>

TCDCA	taurochenodeoxycholic acid	<a href="#">LMST05040005</a>
CDCA-3S	chenodeoxycholic acid 3-sulfate	<a href="#">LMST05020024</a>
GCDCA-3S	glycochenodeoxycholic acid 3-sulfate	
TCDCA-3S	taurochenodeoxycholic acid 3-sulfate	<a href="#">LMST05020029</a>
GUDCA	glycoursodeoxycholic acid	<a href="#">LMST05030016</a>
TUDCA	tauroursodeoxycholic acid	<a href="#">LMST05040015</a>
UDCA-3S	ursodeoxycholic acid 3-sulfate	<a href="#">LMST05020033</a>
GUDCA-3S	glycoursodeoxycholic acid 3-sulfate	<a href="#">LMST05030012</a>
TUDCA-3S	tauroursodeoxycholic acid 3-sulfate	
DCA-3S	deoxycholic acid 3-sulfate	<a href="#">LMST05020038</a>
GDCA	glycodeoxycholic acid	<a href="#">LMST05030006</a>
TDCA	taurodeoxycholic acid	<a href="#">LMST05040013</a>
GDCA-3S	glycodeoxycholic acid 3-sulfate	
TDCA-3S	taurodeoxycholic acid 3-sulfate	
GLCA	glycolithocholic acid	<a href="#">LMST05030009</a>
TLCA	tauroolithocholic acid	<a href="#">LMST05040003</a>
LCA-3S	lithocholic acid 3-sulfate	<a href="#">LMST05020015</a>
GLCA-3S	glycolithocholic acid 3-sulfate	<a href="#">LMST05030004</a>
TLCA-3S	tauroolithocholic acid 3-sulfate	<a href="#">LMST05020003</a>
GHCA	glycohyocholic acid	
THCA	taurohyocholic acid	<a href="#">LMST05040010</a>
GCA-1 $\beta$ -ol	glyco 1 $\beta$ ,3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (glyco1 $\beta$ -hydroxy cholic acid)	
TCA-1 $\beta$ -ol	tauro 1 $\beta$ ,3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (tauro1 $\beta$ -hydroxy cholic acid)	
CA-1 $\beta$ -ol	1 $\beta$ ,3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (1 $\beta$ -hydroxy cholic acid)	<a href="#">LMST04010114</a>
GCA-6 $\alpha$ -ol	glyco 3 $\alpha$ ,6 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (glyco 6 $\alpha$ -hydroxy cholic acid)	
TCA-6 $\alpha$ -ol	tauro 3 $\alpha$ ,6 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (tauro 6 $\alpha$ -hydroxy cholic acid)	
CA-6 $\alpha$ -ol	3 $\alpha$ ,6 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -tetrahydroxy-5 $\beta$ -cholanoic acid (6 $\alpha$ -hydroxy cholic acid)	<a href="#">LMST04010118</a>
CDCA-1 $\beta$ -ol	1 $\beta$ ,3 $\alpha$ ,7 $\alpha$ -trihydroxy-5 $\beta$ -cholanoic acid (1 $\beta$ -hydroxy chenodeoxycholic acid)	<a href="#">LMST04010058</a>
GCA- $\Delta^4$ -3-one	glyco 7 $\alpha$ ,12 $\alpha$ -dihydroxy-3-oxo-4-cholenoic acid	
TCA- $\Delta^4$ -3-one	tauro 7 $\alpha$ ,12 $\alpha$ -dihydroxy-3-oxo-4-cholenoic acid	
GCDCA- $\Delta^4$ -3-one	glyco 7 $\alpha$ -hydroxy-3-oxo-4-cholenoic acid	<a href="#">LMST05030020</a>

TCDCA- $\Delta^4$ -3-one	tauro 7 $\alpha$ -hydroxy-3-oxo-4-cholenoic acid	
$\Delta^5$ -3 $\beta$ -ol	3 $\beta$ -hydroxy-5-cholenoic acid	<a href="#">LMST04010201</a>
G $\Delta^5$ -3 $\beta$ -ol	glyco 3 $\beta$ -hydroxy-5-cholenoic acid	
T $\Delta^5$ -3 $\beta$ -ol	tauro 3 $\beta$ -hydroxy-5-cholenoic acid	
$\Delta^5$ -3 $\beta$ -ol-3S	3 $\beta$ -hydroxy-5-cholenoic acid 3-sulfate	
G $\Delta^5$ -3 $\beta$ -ol-3S	glyco 3 $\beta$ -hydroxy-5-cholenoic acid 3-sulfate	
T $\Delta^5$ -7 $\alpha$ -ol-3S	tauro 3 $\beta$ -hydroxy-5-cholenoic acid 3-sulfate	
$\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol	3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholenoic acid	<a href="#">LMST04010217</a>
G $\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol	glyco 3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholenoic acid	
T $\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol	tauro 3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholenoic acid	
$\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol-3S	3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholen-24-oic acid 3-sulfate	
G $\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol-3S	glyco 3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholenoic acid 3-sulfate	
T $\Delta^5$ -3 $\beta$ ,7 $\alpha$ -diol-3S	tauro 3 $\beta$ ,7 $\alpha$ -dihydroxy-5-cholenoic acid 3-sulfate	
$\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol	3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholenoic acid	<a href="#">LMST04010227</a>
G $\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol	glyco 3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholenoic acid	
T $\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol	tauro 3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholenoic acid	
$\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol-3S	3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholen-24-oic acid 3-sulfate	
G $\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol-3S	glyco 3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholenoic acid 3-sulfate	
T $\Delta^5$ -3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -triol-3S	tauro 3 $\beta$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy-5-cholenoic acid 3-sulfate	

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