

Supplementary Tables

Supplementary Table 1. Association between demographics and BA concentrations and indices.

BA(μ M) / BA indices (%)	Mixed effect with covariates						Interaction (group \times covariates)		
	Group	Gender	Age continuous	BMI continuous	Age category	BMI category	Gender	BMI continuous	BMI Category
	P-value								
Total BA	0.000	0.207	0.700	0.067	0.772	0.026	NA	NA	0.136
Total LCA	0.000	0.276	0.191	0.121	0.198	0.178	NA	NA	NA
Total UDCA	0.000	0.047	0.562	0.056	0.613	0.023	0.114	0.219	0.096
Total CDCA	0.000	0.965	0.262	0.113	0.425	0.048	NA	NA	0.199
Total CA	0.005	0.193	0.113	0.791	0.201	0.098	NA	NA	NA
Total MCA	0.000	0.892	0.402	0.534	0.441	0.862	NA	NA	NA
Total HCA	0.003	0.226	0.123	0.831	0.209	0.318	NA	NA	NA
% LCA	0.000	0.047	0.392	0.544	0.733	0.448	0.682	NA	NA
% CDCA	0.000	0.043	0.716	0.201	0.652	0.166	0.112	NA	NA
% DCA	0.000	0.830	0.430	0.400	0.249	0.581	NA	NA	NA
% MCA	0.062	0.166	0.569	0.008	0.595	0.004	NA	0.325	0.312
Total Unamidated	0.000	0.429	0.130	0.090	0.222	0.058	NA	NA	NA
Total G-amidated	0.000	0.102	0.902	0.051	0.950	0.025	NA	0.263	0.136
Total T-amidated	0.002	0.349	0.128	0.532	0.249	0.045	NA	NA	0.245
Total Unsulfated	0.000	0.581	0.581	0.936	0.659	0.353	NA	NA	NA
Total Sulfated	0.000	0.156	0.631	0.051	0.716	0.022	NA	0.263	0.139
Total Mono-OH	0.000	0.276	0.191	0.121	0.329	0.124	NA	NA	NA
Total Di-OH	0.000	0.123	0.721	0.046	0.459	0.060	NA	0.236	NA
Total Tri-OH	0.000	0.333	0.307	0.792	0.563	0.279	NA	NA	NA
% Mono-OH	0.000	0.047	0.392	0.544	0.733	0.448	0.777	NA	NA
% Tri-OH	0.019	0.056	0.638	0.135	0.568	0.043	0.308	NA	0.529
Total 12 α -OH	0.000	0.957	0.104	0.384	0.131	0.366	NA	NA	NA
Total non-12 α -OH	0.000	0.152	0.893	0.055	0.959	0.019	NA	NA	0.108
12 α -OH/ non12 α -OH	0.000	0.072	0.549	0.984	0.934	0.598	NA	NA	NA
% 12 α -OH	0.000	0.183	0.649	0.868	0.450	0.951	NA	NA	NA
% non-12 α -OH	0.000	0.183	0.649	0.868	0.450	0.951	NA	NA	NA
Total Primary	0.000	0.842	0.230	0.232	0.368	0.078	NA	NA	NA
Total Secondary	0.000	0.037	0.615	0.040	0.668	0.023	0.128	0.243	0.132
Primary/ Secondary	0.005	0.278	0.675	0.652	0.704	0.217	NA	NA	NA
% Primary	0.000	0.009	0.610	0.613	0.529	0.782	0.046	NA	NA
% Secondary	0.000	0.009	0.610	0.613	0.529	0.782	0.046	NA	NA

NA: Not applicable because of the lack of significance from the mixed effect analysis.

Supplementary Table 2. Full list of BA concentrations and indices in controls vs. patients.

BA (μ M) / BA indices (%)	Controls		Patients		Patients vs. Controls	
	mean	SE	Mean	SE	Ratio	p-value
LCA-S	0.01	0.00	0.03	0.01	4.48	0.00
G-LCA-S	0.78	0.04	2.23	0.20	2.84	0.00
T-LCA-S	0.22	0.01	0.65	0.06	2.96	0.00
UDCA-S	0.45	0.02	1.56	0.23	3.47	0.01
G-UDCA-S	1.04	0.05	15.3	2.68	14.7	0.00
T-UDCA-S	0.03	0.00	1.23	0.27	46.7	0.01
CDCA-S	0.07	0.01	0.19	0.03	2.83	0.00
G-CDCA-S	2.38	0.13	18.7	1.79	7.86	0.00
T-CDCA-S	0.06	0.00	1.91	0.38	34.5	0.00
DCA-S	0.01	0.00	0.04	0.01	6.95	0.04
G-DCA-S	2.90	0.14	4.28	0.54	1.48	0.02
T-DCA-S	0.22	0.02	0.52	0.07	2.35	0.01
CA-S	0.00	0.00	0.08	0.01	19.1	0.00
G-CA-S	0.06	0.01	0.91	0.13	16.1	0.00
T-CA-S	0.13	0.01	1.03	0.21	8.14	0.04
Sulfated BA	8.35	0.31	48.7	4.77	5.83	0.00
Sulfated + Unamidated BA	0.54	0.03	1.90	0.24	3.56	0.00
Sulfated G-BA	7.17	0.28	41.4	4.12	5.78	0.00
Sulfated T-BA	0.65	0.03	5.34	0.74	8.23	0.00
Sulfated U-, G-, T-LCA	1.01	0.05	2.91	0.24	2.88	0.00
Sulfated U-, G-, T-UDCA	1.52	0.07	18.1	3.08	11.9	0.00
Sulfated U-, G-, T-CDCA	2.51	0.13	20.8	2.07	8.31	0.00
Sulfated U-, G-, T-DCA	3.13	0.16	4.84	0.58	1.55	0.01
Sulfated U-, G-, T-CA	0.19	0.01	2.01	0.31	10.8	0.00
Sulfated 12 α -OH BA	3.31	0.16	6.85	0.74	2.07	0.00
Sulfated non-12 α -OH BA	5.04	0.19	41.8	4.31	8.30	0.00
Sulfated primary BA	2.69	0.13	22.8	2.29	8.48	0.00
Sulfated secondary BA	5.66	0.23	25.8	3.36	4.56	0.00
LCA	0.00	0.00	0.00	0.00	32.9	0.00
G-LCA	0.00	0.00	0.00	0.00	3.28	0.93
T-LCA	0.00	0.00	0.00	0.00	0.49	0.66
UDCA	0.00	0.00	0.08	0.03	22.5	0.03
G-UDCA	0.03	0.00	0.41	0.17	12.5	0.06
T-UDCA	0.00	0.00	0.01	0.00	6.73	0.09
CDCA	0.00	0.00	0.02	0.00	4.65	0.01
G-CDCA	0.01	0.00	0.09	0.01	11.7	0.00
T-CDCA	0.00	0.00	0.10	0.02	62.4	0.01
DCA	0.02	0.00	0.04	0.00	1.71	0.01
G-DCA	0.01	0.00	0.04	0.00	3.81	0.00
T-DCA	0.00	0.00	0.01	0.00	3.70	0.01
HDCA	0.01	0.00	0.01	0.00	1.54	0.08
G-HDCA	0.00	0.00	0.00	0.00	7.29	0.09
MDCA	0.06	0.01	0.05	0.01	0.90	0.82
CA	0.18	0.03	0.24	0.03	1.36	0.09
G-CA	0.07	0.00	0.55	0.07	8.24	0.00
T-CA	0.01	0.00	0.32	0.08	35.5	0.10
MCA	0.03	0.00	0.12	0.02	4.27	0.00
G-MCA	0.29	0.02	1.94	0.29	6.74	0.00
T-MCA	0.04	0.00	0.73	0.09	18.0	0.00
HCA	0.01	0.00	0.01	0.00	0.72	0.46
G-HCA	0.02	0.00	0.17	0.02	10.8	0.00
T-HCA	0.00	0.00	0.09	0.02	70.0	0.07
Nor-DCA	0.00	0.00	0.01	0.00	1.21	0.25
12-oxo-CDCA	0.12	0.01	0.52	0.07	4.43	0.00
3-dehydroCA	0.01	0.00	0.29	0.11	19.7	0.01
6-oxo-LCA	0.00	0.00	0.01	0.00	19.1	0.00
7-oxo-LCA	0.00	0.00	0.02	0.00	6.41	0.00
12-oxo-LCA	0.01	0.00	0.01	0.00	0.67	0.33
isoLCA	0.00	0.00	0.01	0.00	176	0.00
isoDCA	0.00	0.00	0.00	0.00	1.49	0.69

Unsulfated BA	0.94	0.05	5.91	0.57	6.26	0.00
Unsulfated + Unamidated BA	0.46	0.04	1.43	0.16	3.08	0.00
Unsulfated G-BA	0.42	0.02	3.20	0.44	7.59	0.00
Unsulfated T-BA	0.06	0.00	1.27	0.15	22.4	0.00
Unsulfated U-, G-, T-LCA	0.00	0.00	0.01	0.00	7.53	0.05
Unsulfated U-, G-, T-UDCA	0.04	0.00	0.50	0.21	13.2	0.05
Unsulfated U-, G-, T-CDCA	0.01	0.00	0.21	0.03	16.4	0.01
Unsulfated U-, G-, T-DCA	0.03	0.00	0.09	0.01	2.48	0.00
Unsulfated U-, G-, T-HDCA	0.01	0.00	0.01	0.00	1.57	0.08
Unsulfated U-, G-, T-MDCA	0.06	0.01	0.05	0.01	0.90	0.82
Unsulfated U-, G-, T-CA	0.25	0.03	1.12	0.14	4.39	0.01
Unsulfated U-, G-, T-MCA	0.36	0.02	2.79	0.34	7.83	0.00
Unsulfated U-, G-, T-HCA	0.03	0.00	0.27	0.04	10.6	0.00
Unsulfated 12 α -OH BA	0.31	0.03	1.50	0.19	4.86	0.00
Unsulfated non-12 α -OH BA	0.63	0.03	4.40	0.50	6.94	0.00
Unsulfated primary BA	0.65	0.04	4.39	0.43	6.76	0.00
Unsulfated secondary BA	0.29	0.02	1.52	0.25	5.17	0.00
Total BA	9.30	0.33	54.6	5.20	5.87	0.00
Total Unamidated BA	1.00	0.05	3.33	0.33	3.34	0.00
Total primary unamidated BA	0.29	0.03	0.66	0.06	2.26	0.00
Total secondary unamidated BA	0.71	0.03	2.68	0.30	3.78	0.00
Total primary amidated BA	3.05	0.15	26.6	2.57	8.71	0.00
Total secondary amidated BA	5.24	0.21	24.7	3.29	4.70	0.00
Total G-BA	7.59	0.29	44.6	4.46	5.88	0.00
Total primary G-BA	2.82	0.14	22.4	2.09	7.94	0.00
Total secondary G-BA	4.77	0.20	22.3	3.07	4.66	0.00
Total T-BA	0.71	0.03	6.61	0.85	9.37	0.00
Total primary T-BA	0.23	0.01	4.19	0.68	17.9	0.00
Total secondary T-BA	0.47	0.02	2.42	0.32	5.13	0.00
Total U-, G-, T-LCA	1.01	0.05	2.92	0.24	2.88	0.00
Total U-, G-, T-UDCA	1.56	0.07	18.6	3.23	11.9	0.00
Total U-, G-, T-CDCA	2.52	0.13	21.0	2.09	8.35	0.00
Total U-, G-, T-DCA	3.16	0.16	4.92	0.58	1.56	0.07
Total U-, G-, T-HDCA	0.01	0.00	0.01	0.00	1.57	0.05
Total U-, G-, T-MDCA	0.06	0.01	0.05	0.01	0.90	0.99
Total U-, G-, T-CA	0.44	0.03	3.13	0.44	7.09	0.00
Total U-, G-, T-MCA	0.36	0.02	2.79	0.34	7.83	0.00
Total U-, G-, T-HCA	0.03	0.00	0.27	0.04	10.6	0.00
Total 12 α -OH BA	3.62	0.17	8.35	0.83	2.30	0.00
Total non-12 α -OH BA	5.67	0.20	46.2	4.68	8.15	0.00
Total primary BA	3.34	0.15	27.2	2.59	8.15	0.00
Total secondary BA	5.95	0.23	27.3	3.52	4.59	0.00
Total Mono-hydroxyl BA	1.01	0.05	2.92	0.24	2.88	0.00
Total Di-hydroxyl BA	7.30	0.29	44.6	4.58	6.11	0.00
Total Tri-hydroxyl BA	0.82	0.04	6.19	0.65	7.52	0.00
%Sulfated BA	88.5%	0.46%	83.0%	0.60%	0.94	0.00
%Sulfation LCA	99.7%	0.05%	99.2%	0.16%	0.99	0.85
%Sulfation UDCA	97.0%	0.16%	97.4%	0.20%	1.00	0.35
%Sulfation CDCA	99.4%	0.04%	98.7%	0.12%	0.99	0.25
%Sulfation DCA	98.3%	0.09%	96.2%	0.35%	0.98	0.01
%Sulfation CA	53.0%	1.22%	52.6%	1.05%	0.99	0.97
%Sulfation on mono-hydroxy	99.7%	0.05%	99.2%	0.16%	0.99	0.85
%Sulfation on dihydroxy	97.6%	0.09%	97.4%	0.16%	1.00	0.23
%Sulfation on tri-hydroxy	26.7%	0.77%	26.5%	0.81%	0.99	0.85
%Sulfation on primary BA	79.2%	0.66%	76.8%	0.68%	0.97	0.93
%Sulfation on secondary BA	93.3%	0.41%	86.9%	0.76%	0.93	0.00
%Sulfation on 12 α -OH BA	87.1%	0.85%	75.9%	0.95%	0.87	0.00
%Sulfation on non-12 α -OH BA	87.8%	0.43%	84.2%	0.60%	0.96	0.06
% Sulfation on unamidated BA	58.0%	1.02%	49.6%	1.08%	0.85	0.00
%Sulfation on amidated BA	93.6%	0.23%	88.9%	0.44%	0.95	0.00
%Sulfation on G-BA	93.7%	0.22%	90.2%	0.40%	0.96	0.00
%Sulfation on T-BA	91.5%	0.31%	80.9%	0.78%	0.89	0.00
%Unamidated BA	12.3%	0.47%	13.2%	0.65%	1.07	0.01
% G-Amidated BA	79.7%	0.49%	76.0%	0.71%	0.95	0.00
% T-Amidated BA	8.0%	0.26%	10.8%	0.46%	1.35	0.01
% Amidated BA	87.7%	0.47%	86.8%	0.65%	0.99	0.05

%Amidation LCA	98.7%	0.14%	98.1%	0.21%	0.99	0.39
%Amidation UDCA	68.5%	0.72%	78.0%	0.95%	1.14	0.00
%Amidation CDCA	95.8%	0.28%	97.8%	0.20%	1.02	0.00
%Amidation DCA	98.5%	0.12%	95.9%	0.44%	0.97	0.04
%Amidation CA	71.1%	1.18%	77.2%	1.07%	1.09	0.01
%Amidation MCA	88.9%	0.69%	90.8%	0.75%	1.02	0.94
%Amidation HCA	75.4%	1.12%	92.8%	0.81%	1.23	0.00
%Unamidation LCA	1.31%	0.14%	1.90%	0.21%	1.46	0.39
%G-Amidation LCA	75.6%	0.54%	74.7%	0.81%	0.99	0.84
%T-Amidation LCA	23.1%	0.55%	23.4%	0.80%	1.01	0.99
%Unamidation UDCA	31.5%	0.72%	22.0%	0.95%	0.70	0.00
%G-Amidation UDCA	66.2%	0.72%	70.0%	1.17%	1.06	0.98
%T-Amidation UDCA	2.25%	0.09%	8.08%	0.54%	3.60	0.00
%Unamidation CDCA	4.20%	0.28%	2.21%	0.20%	0.53	0.00
%G-Amidation CDCA	93.1%	0.32%	91.8%	0.43%	0.99	0.55
%T-Amidation CDCA	2.72%	0.10%	6.01%	0.40%	2.21	0.02
%Unamidation DCA	1.53%	0.12%	4.08%	0.44%	2.66	0.04
%G-Amidation DCA	91.6%	0.28%	83.0%	0.81%	0.91	0.00
%T-Amidation DCA	6.88%	0.26%	13.0%	0.72%	1.88	0.00
%Unamidation HDCA	98.7%	0.56%	94.0%	0.85%	0.95	0.04
%G-Amidation HDCA	1.29%	0.56%	5.94%	0.85%	4.62	0.03
%Unamidation CA	28.9%	1.18%	22.8%	1.07%	0.79	0.01
%G-Amidation CA	34.1%	0.88%	52.0%	0.93%	1.53	0.00
%T-Amidation CA	37.0%	1.18%	25.2%	0.94%	0.68	0.00
%Unamidation MCA	11.1%	0.69%	9.23%	0.75%	0.83	0.94
%G-Amidation MCA	78.3%	0.65%	69.7%	0.98%	0.89	0.00
%T-Amidation MCA	10.6%	0.35%	21.1%	0.83%	1.98	0.00
%Unamidation HCA	24.6%	1.12%	7.22%	0.81%	0.29	0.00
%G-Amidation HCA	68.9%	1.10%	76.2%	1.06%	1.11	0.00
%T-Amidation HCA	6.50%	0.27%	16.5%	0.87%	2.54	0.00
%Unamidation on primary BA	9.53%	0.57%	6.41%	0.41%	0.67	0.00
%Unamidation on secondary BA	10.3%	0.29%	9.59%	0.46%	0.93	0.00
%Unamidation on 12 α -OH	9.41%	0.70%	14.2%	0.76%	1.51	0.00
%Unamidation on non-12 α -OH	15.0%	0.48%	12.9%	0.68%	0.86	0.00
%Amidation on monohydroxy	98.7%	0.14%	98.1%	0.21%	0.99	0.39
%Amidation on dihydroxy	90.3%	0.30%	90.8%	0.52%	1.01	0.00
%Amidation on trihydroxy	77.9%	0.97%	83.9%	0.81%	1.08	0.00
%Amidation on primary BA	90.5%	0.57%	93.6%	0.41%	1.03	0.00
%Amidation on secondary BA	85.7%	0.52%	80.0%	0.92%	0.93	0.29
%Amidation on 12 α -OH	90.6%	0.70%	85.8%	0.76%	0.95	0.00
%Amidation on non-12 α -OH	87.9%	0.35%	92.1%	0.39%	1.05	0.00
%G-amidation on monohydroxy	75.6%	0.54%	74.7%	0.81%	0.99	0.84
%T-amidation on monohydroxy	23.1%	0.55%	23.4%	0.80%	1.01	0.99
%G-amidation on dihydroxy	86.0%	0.35%	83.1%	0.68%	0.97	0.00
%T-amidation on dihydroxy	4.32%	0.17%	7.78%	0.40%	1.80	0.12
%G-amidation on trihydroxy	54.1%	0.79%	61.2%	0.78%	1.13	0.00
%T-amidation on trihydroxy	23.8%	0.74%	22.8%	0.78%	0.96	0.58
%G-amidation on primary BA	82.1%	0.63%	83.2%	0.53%	1.01	0.01
%G-amidation on secondary BA	77.6%	0.53%	68.6%	0.97%	0.88	0.05
%G-amidation on 12 α -OH	80.2%	0.71%	68.8%	0.88%	0.86	0.00
%G-amidation on non-12 α -OH	78.2%	0.51%	77.4%	0.75%	0.99	0.00
%T-amidation on primary BA	8.38%	0.34%	10.4%	0.46%	1.24	0.51
%T-amidation on secondary BA	8.18%	0.28%	11.4%	0.51%	1.39	0.17
%T-amidation on 12 α -OH	10.4%	0.34%	17.0%	0.75%	1.64	0.00
%T-amidation on non-12 α -OH	6.81%	0.22%	9.77%	0.42%	1.43	0.19
%Total Mono-hydroxyl BA: Total BA	11.5%	0.38%	9.16%	0.39%	0.79	0.00
%Total Di-hydroxyl BA: Total BA	76.6%	0.50%	72.6%	0.65%	0.95	0.00
%Total Tri-hydroxyl BA: Total BA	9.58%	0.33%	13.1%	0.43%	1.37	0.00
%12 α -OH: Total BA	36.7%	0.62%	22.1%	0.54%	0.60	0.00
%non-12 α -OH: Total BA	63.3%	0.62%	77.9%	0.54%	1.23	0.00
% Primary BA: Total BA	36.7%	0.70%	49.4%	1.06%	1.35	0.00
%Secondary BA: Total BA	63.3%	0.70%	50.6%	1.06%	0.80	0.00
% Total U-, G-, T-LCA : Total BA	11.5%	0.38%	9.16%	0.39%	0.79	0.00
% Total U-, G-, T-UDCA : Total BA	17.7%	0.49%	21.3%	0.88%	1.21	0.14
% Total U-, G-, T-CDCA : Total BA	27.1%	0.65%	36.3%	0.94%	1.34	0.00
% Total U-, G-, T-DCA : Total BA	31.1%	0.68%	14.6%	0.53%	0.47	0.00

% Total U-, G-, T-HDCA : Total BA	0.07%	0.01%	0.04%	0.00%	0.54	0.05
% Total U-, G-, T-MDCA : Total BA	0.64%	0.04%	0.36%	0.05%	0.56	0.14
% Total U-, G-, T-CA : Total BA	5.25%	0.27%	6.27%	0.25%	1.19	0.06
% Total U-, G-, T-MCA : Total BA	4.03%	0.16%	6.39%	0.34%	1.58	0.00
% Total U-, G-, T-HCA : Total BA	0.30%	0.02%	0.45%	0.04%	1.52	0.02
%LCA: Unamidated BA	0.91%	0.05%	1.41%	0.10%	1.55	0.03
%UDCA: Unamidated BA	50.1%	1.03%	38.1%	1.11%	0.76	0.00
%CDCA: Unamidated BA	6.70%	0.26%	6.85%	0.43%	1.02	0.16
%DCA: Unamidated BA	3.30%	0.13%	4.08%	0.23%	1.23	0.02
%HDCA: Unamidated BA	0.71%	0.07%	0.52%	0.07%	0.73	0.49
%MDCA: Unamidated BA	6.97%	0.39%	4.47%	0.31%	0.64	0.02
%CA: Unamidated BA	13.6%	0.72%	13.0%	0.60%	0.96	0.28
%MCA: Unamidated BA	2.98%	0.16%	4.20%	0.31%	1.41	0.00
%HCA: Unamidated BA	0.93%	0.10%	0.40%	0.14%	0.44	0.02
%G,T-LCA: Amidated BA	13.0%	0.42%	10.9%	0.48%	0.84	0.00
%G,T-UDCA: Amidated BA	14.5%	0.53%	19.4%	0.88%	1.33	0.02
%G,T-CDCA: Amidated BA	29.8%	0.72%	40.5%	0.96%	1.36	0.00
%G,T-DCA: Amidated BA	34.7%	0.73%	16.5%	0.58%	0.47	0.00
%G,T-HDCA: Amidated BA	0.00%	0.00%	0.00%	0.00%	3.43	0.09
%G,T-CA: Amidated BA	3.48%	0.12%	5.46%	0.24%	1.57	0.00
%G,T-MCA: Amidated BA	4.21%	0.18%	6.91%	0.36%	1.64	0.00
%G,T-HCA: Amidated BA	0.23%	0.01%	0.44%	0.03%	1.91	0.03
%G-LCA: G-Amidated BA	11.1%	0.38%	9.98%	0.49%	0.90	0.00
%G-UDCA: G-Amidated BA	15.4%	0.54%	19.0%	0.89%	1.24	0.02
%G-CDCA: G-Amidated BA	31.8%	0.74%	43.6%	1.02%	1.37	0.00
%G-DCA: G-Amidated BA	35.6%	0.75%	16.7%	0.59%	0.47	0.00
%G-HDCA: G-Amidated BA	0.00%	0.00%	0.00%	0.00%	3.61	0.08
%G-CA: G-Amidated BA	1.83%	0.08%	4.23%	0.22%	2.31	0.00
%G-MCA: G-Amidated BA	4.10%	0.17%	6.06%	0.31%	1.48	0.01
%G-HCA: G-Amidated BA	0.23%	0.01%	0.39%	0.03%	1.69	0.09
%T-LCA: T-Amidated BA	32.2%	0.78%	19.9%	0.79%	0.62	0.00
%T-UDCA: T-Amidated BA	5.28%	0.26%	16.5%	0.94%	3.12	0.00
%T-CDCA: T-Amidated BA	10.0%	0.37%	18.8%	0.79%	1.88	0.00
%T-DCA: T-Amidated BA	26.3%	0.67%	15.5%	0.61%	0.59	0.00
%T-CA: T-Amidated BA	20.5%	0.60%	15.5%	0.63%	0.76	0.04
%T-MCA: T-Amidated BA	5.48%	0.25%	13.2%	0.73%	2.40	0.00
%T-HCA: T-Amidated BA	0.24%	0.01%	0.62%	0.06%	2.59	0.02
%Sulfated LCA : Sulfated BA	12.9%	0.42%	11.1%	0.46%	0.86	0.00
%Sulfated UDCA : Sulfated BA	19.7%	0.58%	24.7%	0.93%	1.25	0.25
%Sulfated CDCA : Sulfated BA	30.7%	0.73%	43.5%	1.04%	1.42	0.00
%Sulfated DCA : Sulfated BA	34.2%	0.70%	17.1%	0.59%	0.50	0.00
%Sulfated CA : Sulfated BA	2.42%	0.09%	3.57%	0.16%	1.48	0.00
%Unsulfated LCA : unsulfated BA	0.16%	0.02%	0.18%	0.02%	1.09	0.02
%Unsulfated UDCA : unsulfated BA	4.53%	0.20%	5.12%	0.47%	1.13	0.63
%Unsulfated CDCA : unsulfated BA	1.60%	0.07%	3.12%	0.24%	1.95	0.01
%Unsulfated DCA : unsulfated BA	5.01%	0.18%	2.81%	0.17%	0.56	0.00
%Unsulfated HDCA : unsulfated BA	0.84%	0.07%	0.33%	0.04%	0.39	0.00
%Unsulfated MDCA : unsulfated BA	7.15%	0.34%	2.63%	0.21%	0.37	0.00
%Unsulfated CA : unsulfated BA	22.1%	0.77%	21.62%	0.77%	0.98	0.89
%Unsulfated MCA : unsulfated BA	40.5%	0.90%	38.84%	1.18%	0.96	0.81
%Unsulfated HCA : unsulfated BA	3.39%	0.19%	3.74%	0.28%	1.10	0.66
%Primary unamidated BA:Total BA	3.55%	0.27%	2.61%	0.19%	0.74	0.07
%Secondary unamidated BA:Total BA	8.8%	0.32%	10.5%	0.58%	1.20	0.02
%Primary amidated BA:Total BA	33.1%	0.68%	46.8%	1.06%	1.41	0.00
%Secondary amidated BA:Total BA	54.6%	0.71%	40.0%	0.96%	0.73	0.00
%Primary G-BA:Total BA	30.4%	0.67%	40.8%	0.90%	1.34	0.00
%Secondary G-BA:Total BA	49.3%	0.66%	35.2%	0.93%	0.71	0.00
%Primary T-BA:Total BA	2.73%	0.10%	6.00%	0.35%	2.20	0.00
%Secondary T-BA:Total BA	5.25%	0.19%	4.81%	0.22%	0.92	0.00
%Unamidated -Unsulfated BA: Total BA	6.03%	0.38%	7.57%	0.48%	1.25	0.53
%Amidated -Unsulfated G-BA : Total BA	4.86%	0.16%	7.04%	0.28%	1.45	0.00
%Amidated -Unsulfated T-BA : Total BA	0.65%	0.03%	2.42%	0.17%	3.73	0.00
%Amidated -Unsulfated BA: Total BA	5.50%	0.19%	9.46%	0.38%	1.72	0.00
% Unamidated: Unsulfated BA	44.5%	1.01%	36.9%	1.20%	0.83	0.00
%Amidated G: Unsulfated BA	48.7%	0.88%	47.8%	0.94%	0.98	0.57
%Amidated T: Unsulfated BA	6.74%	0.24%	15.3%	0.71%	2.26	0.00

% Amidated: Unsulfated BA	55.5%	1.01%	63.1%	1.20%	1.14	0.00
%Unamidated -Sulfated BA: Total BA	6.27%	0.20%	5.58%	0.31%	0.89	0.00
%Amidated -Sulfated G-BA : Total BA	74.9%	0.54%	69.0%	0.76%	0.92	0.57
%Amidated -Sulfated T-BA : Total BA	7.33%	0.24%	8.39%	0.36%	1.15	0.33
%Amidated -Sulfated BA: Total BA	82.2%	0.53%	77.4%	0.72%	0.94	0.29
% Unamidated: BA-Sulfates	7.29%	0.25%	7.33%	0.44%	1.01	0.00
% Amidated G: BA-Sulfates	84.4%	0.35%	82.5%	0.61%	0.98	0.00
%Amidated T: BA-sulfates	8.28%	0.27%	10.1%	0.43%	1.22	0.66
% Amidated: BA-Sulfates	92.7%	0.25%	92.7%	0.44%	1.00	0.00
%Unsulfated LCA: Total BA	0.01%	0.00%	0.03%	0.00%	1.90	0.09
%Unsulfated UDCA: Total BA	0.48%	0.04%	0.52%	0.05%	1.09	0.90
%Unsulfated CDCA: Total BA	0.15%	0.01%	0.42%	0.04%	2.76	0.00
%Unsulfated DCA: Total BA	0.43%	0.02%	0.38%	0.02%	0.87	0.02
%Unsulfated HDCA: Total BA	0.07%	0.01%	0.04%	0.00%	0.54	0.00
%Unsulfated MDCA: Total BA	0.64%	0.04%	0.36%	0.05%	0.56	0.14
%Unsulfated CA: Total BA	3.15%	0.26%	3.36%	0.20%	1.07	0.95
%Unsulfated MCA: Total BA	4.03%	0.16%	6.39%	0.34%	1.58	0.00
%Unsulfated HCA: Total BA	0.30%	0.02%	0.45%	0.04%	1.52	0.12
%Unsulfated Mono-hydroxyl BA: Total BA	0.01%	0.00%	0.03%	0.00%	1.90	0.09
%Unsulfated Di-hydroxyl BA: Total BA	1.78%	0.06%	1.72%	0.09%	0.97	0.10
%Unsulfated Tri-hydroxyl BA: Total BA	7.48%	0.31%	10.2%	0.39%	1.36	0.00
% Unsulfated primary: Total BA	7.63%	0.32%	10.6%	0.40%	1.39	0.00
% Unsulfated Secondary: Total BA	3.91%	0.24%	6.40%	0.43%	1.64	0.05
% Unsulfated 12 α -OH: Total BA	3.85%	0.27%	4.94%	0.29%	1.28	0.04
% Unsulfated non 12 α -OH: Total BA	7.69%	0.29%	12.1%	0.47%	1.57	0.00
%Sulfated LCA: Total BA	11.5%	0.38%	9.13%	0.39%	0.79	0.00
%Sulfated UDCA: Total BA	17.2%	0.48%	20.8%	0.86%	1.21	0.32
%Sulfated CDCA: Total BA	26.9%	0.64%	35.9%	0.93%	1.33	0.00
%Sulfated DCA: Total BA	30.7%	0.68%	14.2%	0.52%	0.46	0.00
%Sulfated CA: Total BA	2.11%	0.07%	2.91%	0.13%	1.38	0.00
%Sulfated Mono-hydroxyl BA: Total BA	11.5%	0.38%	9.13%	0.39%	0.79	0.00
%Sulfated Di-hydroxyl BA: Total BA	74.8%	0.53%	70.9%	0.67%	0.95	0.46
%Sulfated Tri-hydroxyl BA: Total BA	2.11%	0.07%	2.91%	0.13%	1.38	0.00
% Sulfated primary: Total BA	29.0%	0.64%	38.8%	0.98%	1.34	0.00
% Sulfated Secondary: Total BA	59.4%	0.75%	44.2%	1.02%	0.74	0.00
% Sulfated 12 α -OH: Total BA	32.8%	0.69%	17.1%	0.52%	0.52	0.00
% Sulfated non 12 α -OH: Total BA	55.6%	0.62%	65.9%	0.71%	1.18	0.00
% Unsulfated Nor-DCA	0.05%	0.00%	0.03%	0.00%	0.55	0.00
% Unsulfated 12-oxo-CDCA	1.71%	0.19%	3.53%	0.35%	2.07	0.33
% Unsulfated 3-dehydroCA	0.21%	0.02%	1.18%	0.16%	5.52	0.00
% Unsulfated 6-oxo-LCA	0.00%	0.00%	0.06%	0.01%	17.2	0.00
% Unsulfated 7-oxo-LCA	0.03%	0.00%	0.09%	0.02%	3.55	0.06
% Unsulfated 12-oxo-LCA	0.24%	0.09%	0.06%	0.01%	0.26	0.13
% Unsulfated isoLCA	0.00%	0.00%	0.11%	0.02%	189	0.02
% Unsulfated isoDCA	0.03%	0.00%	0.02%	0.00%	0.72	0.06
Primary BA/Secondary BA	0.69	0.03	2.52	0.22	3.63	0.00
Total amidated/total unamidated	12.3	0.51	29.8	2.14	2.42	0.00
12 α -OH/non12 α -OH	0.65	0.02	0.33	0.01	0.51	0.00
CA/CDCA	0.24	0.01	0.24	0.02	1.00	0.63
CA+DCA/CDCA+LCA	1.15	0.04	0.60	0.03	0.52	0.00
Total BA for HI	0.40	0.03	2.92	0.33	7.30	0.00
HI	-0.01	0.01	-0.12	0.01	17.6	0.00

Supplementary Table 3. Area under the ROC curve (AUC) of BA concentrations and indices*.

BA (μM) / BA indices (%)	AUC
Total BA	0.736
Total LCA	0.583
Total UDCA	0.662
Total CDCA	0.770
Total DCA	0.514
Total HDCA	0.659
Total MDCA	0.576
Total CA	0.747
Total MCA	0.691
Total HCA	0.623
% LCA	0.672
% UDCA	0.555
% CDCA	0.677
% DCA	0.812
% HDCA	0.742
% MDCA	0.811
% CA	0.554
% MCA	0.540
% HCA	0.579
Total Unamidated	0.592
Total G-amidated	0.736
Total T-amidated	0.690
% Amidation	0.679
% G-amidation	0.590
% T-amidation	0.507
Total Unsulfated	0.771
Total Sulfated	0.724
% Sulfation	0.581
Total Mono-OH	0.583
Total Di-OH	0.726
Total Tri-OH	0.767
% Mono-OH	0.672
% Di-OH	0.502
% Tri-OH	0.603
Total 12α-OH	0.599
Total non-12α-OH	0.769
12α-OH/ non12α-OH	0.794
CA/ CDCA	0.565
% 12α-OH	0.794
% non-12α-OH	0.794
Total Primary	0.776
Total Secondary	0.626
Primary/ Secondary	0.708
% Primary	0.708
% Secondary	0.708

* AUC from ROC analysis of pooled patients vs. controls.

Supplementary Table 4. Area under the ROC curve (AUC) of the full list BA concentrations and indices*.

BA (μM) / BA indices (%)	AUC
LCA-S	0.526
G-LCA-S	0.572
T-LCA-S	0.564
UDCA-S	0.560
G-UDCA-S	0.702
T-UDCA-S	0.664
CDCA-S	0.511
G-CDCA-S	0.770
T-CDCA-S	0.716
DCA-S	0.678
G-DCA-S	0.524
T-DCA-S	0.537
CA-S	0.690
G-CA-S	0.809
T-CA-S	0.594
Sulfated BA	0.724
Sulfated + Unamidated BA	0.512
Sulfated G-BA	0.729
Sulfated T-BA	0.666
Sulfated U-, G-, T-LCA	0.583
Sulfated U-, G-, T-UDCA	0.662
Sulfated U-, G-, T-CDCA	0.770
Sulfated U-, G-, T-DCA	0.515
Sulfated U-, G-, T-CA	0.728
Sulfated 12 α -OH BA	0.555
Sulfated non-12 α -OH BA	0.765
Sulfated primary BA	0.771
Sulfated secondary BA	0.605
LCA	0.531
G-LCA	0.658
T-LCA	0.640
UDCA	0.519
G-UDCA	0.590
T-UDCA	0.619
CDCA	0.633
G-CDCA	0.690
T-CDCA	0.616
DCA	0.527
G-DCA	0.544

T-DCA	0.611
HDCA	0.657
G-HDCA	0.505
T-HDCA	0.501
MDCA	0.576
CA	0.540
G-CA	0.793
T-CA	0.674
MCA	0.513
G-MCA	0.663
T-MCA	0.711
HCA	0.769
G-HCA	0.646
T-HCA	0.504
Nor-DCA	0.672
12-oxo-CDCA	0.549
3-dehydroCA	0.596
6-oxo-LCA	0.605
7-oxo-LCA	0.581
12-oxo-LCA	0.499
isoLCA	0.517
isoDCA	0.663
Unulfated BA	0.771
Unulfated + Unamidated BA	0.638
Unulfated G-BA	0.760
Unulfated T-BA	0.746
Unulfated U-, G-, T-LCA	0.590
Unulfated U-, G-, T-UDCA	0.603
Unulfated U-, G-, T-CDCA	0.692
Unulfated U-, G-, T-DCA	0.540
Unulfated U-, G-, T-HDCA	0.659
Unulfated U-, G-, T-MDCA	0.424
Unulfated U-, G-, T-CA	0.736
Unulfated U-, G-, T-MCA	0.691
Unulfated U-, G-, T-HCA	0.623
Unulfated 12 α -OH BA	0.769
Unulfated non-12 α -OH BA	0.745
Unulfated primary BA	0.759
Unulfated secondary BA	0.670
Total BA	0.736
Total Unamidated BA	0.592
Total primary unamidated BA	0.593
Total secondary unamidated BA	0.574

Total primary amidated BA	0.780
Total secondary amidated BA	0.613
Total G-BA	0.736
Total primary G-BA	0.782
Total secondary G-BA	0.605
Total T-BA	0.690
Total primary T-BA	0.713
Total secondary T-BA	0.614
Total U-, G-, T-LCA	0.583
Total U-, G-, T-UDCA	0.662
Total U-, G-, T-CDCA	0.770
Total U-, G-, T-DCA	0.514
Total U-, G-, T-HDCA	0.659
Total U-, G-, T-MDCA	0.576
Total U-, G-, T-CA	0.747
Total U-, G-, T-MCA	0.691
Total U-, G-, T-HCA	0.623
Total 12 α -OH BA	0.599
Total non-12 α -OH BA	0.769
Total primary BA	0.776
Total secondary BA	0.626
Total Mono-hydroxyl BA	0.583
Total Di-hydroxyl BA	0.726
Total Tri-hydroxyl BA	0.767
%Sulfated BA	0.581
%Sulfation LCA	0.610
%Sulfation UDCA	0.600
%Sulfation CDCA	0.552
%Sulfation DCA	0.479
%Sulfation CA	0.514
%Sulfation on mono-hydroxy	0.610
%Sulfation on dihydroxy	0.635
%Sulfation on tri-hydroxy	0.484
%Sulfation on primary BA	0.514
%Sulfation on secondary BA	0.461
%Sulfation on 12 α -OH BA	0.696
%Sulfation on non-12 α -OH BA	0.506
% Sulfation on unamidated BA	0.621
%Sulfation on amidated BA	0.621
%Sulfation on G-BA	0.573
%Sulfation on T-BA	0.694
%Unamidated BA	0.679
% G-Amidated BA	0.590

% T-Amidated BA	0.507
% Amidated BA	0.679
%Amidation LCA	0.558
%Amidation UDCA	0.856
%Amidation CDCA	0.721
%Amidation DCA	0.529
%Amidation HDCA	0.497
%Amidation CA	0.636
%Amidation MCA	0.671
%Amidation HCA	0.831
%Unamidation LCA	0.442
%G-Amidation LCA	0.545
%T-Amidation LCA	0.448
%Unamidation UDCA	0.856
%G-Amidation UDCA	0.820
%T-Amidation UDCA	0.536
%Unamidation CDCA	0.279
%G-Amidation CDCA	0.568
%T-Amidation CDCA	0.522
%Unamidation DCA	0.471
%G-Amidation DCA	0.377
%T-Amidation DCA	0.581
%Unamidation HDCA	0.506
%G-Amidation HDCA	0.494
%T-Amidation HDCA	0.500
%Unamidation CA	0.636
%G-Amidation CA	0.730
%T-Amidation CA	0.619
%Unamidation MCA	0.671
%G-Amidation MCA	0.600
%T-Amidation MCA	0.643
%Unamidation HCA	0.831
%G-Amidation HCA	0.688
%T-Amidation HCA	0.533
%Unamidation on primary BA	0.688
%Unamidation on secondary BA	0.747
%Unamidation on 12 α -OH	0.575
%Unamidation on non-12 α -OH	0.780
%Amidation on monohydroxy	0.558
%Amidation on dihydroxy	0.777
%Amidation on trihydroxy	0.657
%Amidation on primary BA	0.688
%Amidation on secondary BA	0.590

%Amidation on 12 α -OH	0.575
%Amidation on non-12 α -OH	0.826
%G-amidation on monohydroxy	0.545
%T-amidation on monohydroxy	0.448
%G-amidation on dihydroxy	0.679
%T-amidation on dihydroxy	0.511
%G-amidation on trihydroxy	0.614
%T-amidation on trihydroxy	0.477
%G-amidation on primary BA	0.571
%G-amidation on secondary BA	0.517
%G-amidation on 12 α -OH	0.663
%G-amidation on non-12 α -OH	0.694
%T-amidation on primary BA	0.499
%T-amidation on secondary BA	0.490
%T-amidation on 12 α -OH	0.557
%T-amidation on non-12 α -OH	0.497
%Total Mono-hydroxyl BA: Total BA	0.672
%Total Di-hydroxyl BA: Total BA	0.502
%Total Tri-hydroxyl BA: Total BA	0.603
%12 α -OH: Total BA	0.794
%non-12 α -OH: Total BA	0.794
% Primary BA: Total BA	0.708
%Secondary BA: Total BA	0.708
% Total U-, G-, T-LCA : Total BA	0.672
% Total U-, G-, T-UDCA : Total BA	0.555
% Total U-, G-, T-CDCA : Total BA	0.677
% Total U-, G-, T-DCA : Total BA	0.812
% Total U-, G-, T-HDCA : Total BA	0.742
% Total U-, G-, T-MDCA : Total BA	0.811
% Total U-, G-, T-CA : Total BA	0.554
% Total U-, G-, T-MCA : Total BA	0.540
% Total U-, G-, T-HCA : Total BA	0.579
%LCA: Unamidated BA	0.465
%UDCA: Unamidated BA	0.682
%CDCA: Unamidated BA	0.438
%DCA: Unamidated BA	0.442
%HDCA: Unamidated BA	0.689
%MDCA: Unamidated BA	0.661
%CA: Unamidated BA	0.527
%MCA: Unamidated BA	0.471
%HCA: Unamidated BA	0.818
%G,T-LCA: Amidated BA	0.683
%G,T-UDCA: Amidated BA	0.518

%G,T-CDCA: Amidated BA	0.677
%G,T-DCA: Amidated BA	0.828
%G,T-HDCA: Amidated BA	0.496
%G,T-CA: Amidated BA	0.582
%G,T-MCA: Amidated BA	0.534
%G,T-HCA: Amidated BA	0.454
%G-LCA: G-Amidated BA	0.676
%G-UDCA: G-Amidated BA	0.520
%G-CDCA: G-Amidated BA	0.680
%G-DCA: G-Amidated BA	0.832
%G-HDCA: G-Amidated BA	0.495
%G-CA: G-Amidated BA	0.708
%G-MCA: G-Amidated BA	0.504
%G-HCA: G-Amidated BA	0.450
%T-LCA: T-Amidated BA	0.724
%T-UDCA: T-Amidated BA	0.500
%T-CDCA: T-Amidated BA	0.641
%T-DCA: T-Amidated BA	0.732
%T-HDCA: T-Amidated BA	0.501
%T-CA: T-Amidated BA	0.592
%T-MCA: T-Amidated BA	0.620
%T-HCA: T-Amidated BA	0.582
%Sulfated LCA : Sulfated BA	0.653
%Sulfated UDCA : Sulfated BA	0.471
%Sulfated CDCA : Sulfated BA	0.707
%Sulfated DCA : Sulfated BA	0.809
%Sulfated CA : Sulfated BA	0.573
%Unsulfated LCA : unsulfated BA	0.622
%Unsulfated UDCA : unsulfated BA	0.684
%Unsulfated CDCA : unsulfated BA	0.474
%Unsulfated DCA : unsulfated BA	0.741
%Unsulfated HDCA : unsulfated BA	0.753
%Unsulfated MDCA : unsulfated BA	0.817
%Unsulfated CA : unsulfated BA	0.479
%Unsulfated MCA : unsulfated BA	0.522
%Unsulfated HCA : unsulfated BA	0.632
%Primary unamidated BA:Total BA	0.640
%Secondary unamidated BA:Total BA	0.692
%Primary amidated BA:Total BA	0.717
%Secondary amidated BA:Total BA	0.695
%Primary G-BA:Total BA	0.711
%Secondary G-BA:Total BA	0.684
%Primary T-BA:Total BA	0.577

%SecondaryT-BA:Total BA	0.663
%Unamidated -Unsulfated BA: Total BA	0.595
%Amidated -Unsulfated G-BA : Total BA	0.580
%Amidated -Unsulfated T-BA : Total BA	0.632
%Amidated -Unsulfated BA: Total BA	0.625
% Unamidated: Unsulfated BA	0.660
%Amidated G: Unsulfated BA	0.543
%Amidated T: Unsulfated BA	0.631
% Amidated: Unsulfated BA	0.660
%Unamidated -Sulfated BA: Total BA	0.765
%Amidated -Sulfated G-BA : Total BA	0.516
%Amidated -Sulfated T-BA : Total BA	0.576
%Amidated -Sulfated BA: Total BA	0.522
% Unamidated: BA-Sulfates	0.750
% Amidated G: BA-Sulfates	0.670
%Amidated T: BA-sulfates	0.565
% Amidated: BA-Sulfates	0.750
%Unsulfated LCA: Total BA	0.620
%Unsulfated UDCA: Total BA	0.630
%Unsulfated CDCA: Total BA	0.526
%Unsulfated DCA: Total BA	0.673
%Unsulfated HDCA: Total BA	0.742
%Unsulfated MDCA: Total BA	0.811
%Unsulfated CA: Total BA	0.537
%Unsulfated MCA: Total BA	0.540
%Unsulfated HCA: Total BA	0.421
%Unsulfated Mono-hydroxyl BA: Total BA	0.620
%Unsulfated Di-hydroxyl BA: Total BA	0.654
%Unsulfated Tri-hydroxyl BA: Total BA	0.574
% Unsulfated primary: Total BA	0.581
% Unsulfated Secondary: Total BA	0.431
% Unsulfated 12 α -OH: Total BA	0.553
% Unsulfated non 12 α -OH: Total BA	0.562
%Sulfated LCA: Total BA	0.671
%Sulfated UDCA: Total BA	0.447
%Sulfated CDCA: Total BA	0.676
%Sulfated DCA: Total BA	0.813
%Sulfated CA: Total BA	0.550
%Sulfated Mono-hydroxyl BA: Total BA	0.671
%Sulfated Di-hydroxyl BA: Total BA	0.506
%Sulfated Tri-hydroxyl BA: Total BA	0.550
% Sulfated primary: Total BA	0.680
% Sulfated Secondary: Total BA	0.717

% Sulfated 12α-OH: Total BA	0.799
% Sulfated non 12α-OH: Total BA	0.711
% Unsulfated Nor-DCA	0.763
% Unsulfated 12-oxo-CDCA	0.409
% Unsulfated 3-dehydroCA	0.498
% Unsulfated 6-oxo-LCA	0.600
% Unsulfated 7-oxo-LCA	0.542
% Unsulfated 12-oxo-LCA	0.478
% Unsulfated isoLCA	0.517
% Unsulfated isoDCA	0.684
Primary BA/Secondary BA	0.708
Total amidated/total unamidated	0.678
12α-OH/non12α-OH	0.794
CA/CDCA	0.565
CA+DCA/CDCA+LCA	0.790
Total BA for HI	0.770
HI	0.664

* AUC from ROC analysis of pooled patients vs. controls.

Supplementary Table 5. ROC analysis of BA concentrations and indices with AUC > 0.7*.

BA (μM) / BA indices (%)	AUC	(Cutoff Value; Sensitivity, Specificity)		
Total BA	0.736	(9.34; 70, 61)	(10.2; 67, 66)	(10.9; 64, 70)
Total CDCA	0.770	(2.66; 72, 70)	(2.74; 71, 71)	(2.88; 70, 73)
Total CA	0.747	(0.43; 70, 69)	(0.44; 69, 69)	(0.45; 69, 70)
% DCA	0.812	(19.5; 81, 70)	(22.1; 75, 75)	(24.3; 70, 81)
% HDCA	0.742	(0.003; 75, 70)	(0.01; 73, 75)	(0.01; 70, 77)
% MDCA	0.811	(0.18; 80, 70)	(0.21; 75, 73)	(0.24; 70, 76)
Total G-amidated	0.736	(7.35; 70, 59)	(8.20; 68, 65)	(8.87; 65, 70)
Total Unsulfated	0.771	(0.96; 71, 70)	(1.00; 71, 71)	(1.04; 70, 73)
Total Sulfated	0.724	(7.71; 70, 56)	(8.72; 68, 64)	(9.63; 65, 70)
Total Di-OH	0.726	(6.90; 70, 59)	(7.51; 67, 64)	(8.39; 65, 70)
Total Tri-OH	0.767	(0.82; 72, 70)	(0.85; 71, 72)	(0.88; 70, 74)
Total non-12α-OH	0.769	(6.38; 70, 69)	(6.43; 69, 69)	(6.57; 69, 70)
12α-OH/ non12α-OH	0.794	(0.37; 78, 70)	(0.41; 76, 76)	(0.45; 70, 78)
% 12α-OH	0.794	(27.1; 78, 70)	(29.1; 76, 76)	(30.9; 70, 78)
% non-12α-OH	0.794	(69.1; 78, 70)	(70.9; 76, 76)	(72.9; 70, 78)
Total Primary	0.776	(3.75; 72, 70)	(4.03; 71, 73)	(4.19; 70, 75)
Primary/ Secondary	0.708	(0.60; 70, 58)	(0.66; 67, 64)	(0.74; 64, 70)
% Primary	0.708	(37.4; 70, 58)	(39.9; 67, 64)	(42.6; 64, 70)
% Secondary	0.708	(57.4; 70, 64)	(60.0; 64, 67)	(62.6; 58, 70)

* AUC from ROC analysis of pooled patients vs. controls.

Supplementary Table 6. Univariate logistic regression analysis of non-BA parameters.

Non-BA parameters	B-value (Regression Coefficient)	P-value	Exp(B)-Odds ratio		
			1 unit change	10% change	20% change
Creatinine (mg/dL)	0.852	0.085	2.34	1.08	1.16
Albumin (g/dL)	-1.616	0.000	0.19	0.53	0.28
INR	5.573	0.000	263	1.74	3.02
Protime (sec)	-0.063	0.002	0.94	0.92	0.85
AST (U/L)	0.141	0.000	1.15	1.38	1.90
ALT (U/L)	0.100	0.000	1.11	1.23	1.52
Bilirubin (mg/dL)	1.775	0.000	5.89	1.12	1.25
AST/ALT	0.542	0.064	1.72	1.06	1.13
MELD	0.470	0.000	1.59	1.39	1.95

Supplementary Table 7. Non- BA parameters in controls and patients with specific liver disease subtype.

Non-BA parameters	Controls		Hepatitis C		Hepatitis B		Laennec Cirrhosis		Primary biliary cholangitis		Primary sclerosing cholangitis		Autoimmune Hepatitis		α-1 antitrypsin deficiency		NASH		Carcinoma		Cryptogenic cirrhosis		Elevated LFT	
	N=103		N=71		N=15		N=117		N=12		N=17		N=27		N=6		N=56		N=26		N=11		N=22	
	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE
Creatinine (mg/dL)	0.87	0.17	0.99	0.06	1.08 ^a	0.08	1.00 ^a	0.05	0.90	0.04	0.96	0.06	0.83	0.03	1.01	0.04	0.95	0.04	0.93	0.05	2.47 ^a	1.47	0.88	0.07
Albumin (g/dL)	3.96	0.30	3.48 ^a	0.06	3.84	0.14	3.37 ^a	0.05	3.61 ^a	0.09	3.51 ^a	0.10	3.42 ^a	0.08	3.48 ^a	0.28	3.64 ^a	0.06	3.50 ^a	0.09	3.18 ^a	0.11	3.70 ^a	0.14
INR	0.99	0.20	1.17 ^a	0.04	1.17	0.17	1.25 ^a	0.03	0.97	0.03	1.16 ^a	0.08	1.20 ^a	0.09	1.45 ^a	0.15	1.14 ^a	0.02	1.22 ^a	0.05	1.36 ^a	0.07	1.12	0.08
Protine (sec)	13.4	1.89	8.20 ^a	0.70	2.30 ^a	1.26	11.4 ^a	0.56	10.8 ^a	0.93	8.09 ^a	1.29	9.30 ^a	1.07	7.22 ^a	2.99	10.1 ^a	0.67	10.0 ^a	1.07	13.8	1.71	8.40 ^a	1.57
AST (U/L)	22.8	6.23	68.4 ^a	7.19	29.9 ^a	3.59	55.6 ^a	4.34	48.4 ^a	8.21	59.5 ^a	8.38	71.8 ^a	9.25	40.5 ^a	7.90	49.8 ^a	4.14	61.0 ^a	7.23	58.3 ^a	6.88	64.4 ^a	13.1
ALT (U/L)	21.0	8.58	57.5 ^a	5.58	28.5 ^a	2.81	45.6 ^a	4.12	46.3 ^a	8.57	58.5 ^a	9.41	76.4 ^a	10.6	28.3 ^a	4.07	55.2 ^a	6.67	51.8 ^a	7.20	37.0 ^a	3.90	72.0 ^a	12.7
Bilirubin (mg/dL)	0.62	0.47	1.46 ^a	0.14	0.88	0.17	2.10 ^a	0.19	1.14	0.14	1.82 ^a	0.44	1.59 ^a	0.19	1.38 ^a	0.18	1.31 ^a	0.11	1.43 ^a	0.19	2.51 ^a	0.56	1.39 ^a	0.36
AST/ALT	1.15	0.26	1.24	0.05	1.07	0.07	1.38 ^a	0.04	1.24	0.11	1.10	0.08	1.26	0.09	1.41	0.14	1.12	0.05	1.27	0.07	1.61 ^a	0.12	0.96 ^a	0.11
MELD	7.13	1.72	10.1 ^a	0.56	13.5 ^a	2.04	11.8 ^a	0.43	8.03	0.47	10.6 ^a	0.91	9.94 ^a	0.75	12.6 ^a	1.74	9.81 ^a	0.47	10.3 ^a	0.65	13.2 ^a	1.36	9.37 ^a	1.31
APRI	NA	NA	1.45	0.20	0.24	0.06	1.24	0.12	0.65	0.15	0.79	0.17	0.85	0.12	0.59	0.27	0.73	0.07	1.43	0.30	1.13	0.22	1.04	0.32

^a Significant difference between controls and each specific liver disease subtype (P<0.05)

Supplementary Table 8. Association between non-BA parameters and BA concentrations and indices.

Non-BA parameters vs.BA/BA indices	AST	ALT	AST/ALT	Bilirubin	Albumin	INR	Protime	Creatinine	APRI	MELD
	P-value									
Total BA	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.614	0.000	0.000
Total LCA	0.000	0.001	0.000	0.000	0.000	0.066	0.008	0.900	0.003	0.001
Total UDCA	0.000	0.000	0.088	0.352	0.000	0.312	0.120	0.754	0.258	0.328
Total CDCA	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.643	0.000	0.000
Total DCA	0.000	0.000	0.127	0.134	0.004	0.749	0.925	0.919	0.020	0.946
Total HDCA	0.003	0.008	0.313	0.225	0.257	0.645	0.241	0.599	0.545	0.367
Total MDCA	0.012	0.361	0.006	0.001	0.012	0.781	0.607	0.928	0.561	0.112
Total CA	0.000	0.032	0.000	0.000	0.000	0.000	0.003	0.649	0.007	0.000
Total MCA	0.000	0.000	0.008	0.117	0.000	0.081	0.168	0.517	0.003	0.054
Total HCA	0.000	0.243	0.000	0.000	0.000	0.000	0.000	0.716	0.001	0.000
% LCA	0.000	0.001	0.051	0.003	0.000	0.049	0.996	0.768	0.046	0.000
% UDCA	0.519	0.470	0.126	0.013	0.001	0.001	0.799	0.831	0.008	0.000
% CDCA	0.001	0.379	0.000	0.000	0.000	0.000	0.000	0.574	0.000	0.000
% DCA	0.001	0.141	0.000	0.000	0.000	0.000	0.003	0.001	0.042	0.000
% HDCA	0.044	0.203	0.155	0.126	0.230	0.144	0.877	0.696	0.239	0.052
% MDCA	0.562	0.700	0.395	0.180	0.103	0.013	0.001	0.788	0.258	0.000
% CA	0.004	0.057	0.558	0.000	0.000	0.031	0.813	0.656	0.125	0.000
% MCA	0.126	0.085	0.682	0.093	0.565	0.924	0.880	0.314	0.505	0.548
% HCA	0.095	0.850	0.007	0.000	0.000	0.002	0.027	0.600	0.012	0.000
Total Unamidated	0.000	0.011	0.004	0.037	0.000	0.069	0.084	0.743	0.046	0.009
Total G-amidated	0.000	0.000	0.000	0.000	0.000	0.002	0.003	0.650	0.000	0.000
Total T-amidated	0.000	0.030	0.000	0.000	0.000	0.000	0.000	0.658	0.000	0.000
% Amidation	0.000	0.009	0.006	0.002	0.000	0.005	0.002	0.157	0.002	0.006
% G-amidation	0.710	0.169	0.265	0.007	0.957	0.910	0.458	0.113	0.582	0.152
% T-amidation	0.000	0.244	0.000	0.000	0.000	0.000	0.002	0.373	0.000	0.000
Total Unsulfated	0.000	0.000	0.000	0.000	0.000	0.002	0.006	0.616	0.000	0.000
Total Sulfated	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.628	0.000	0.000
% Sulfation	0.660	0.842	0.596	0.766	0.255	0.989	0.016	0.276	0.420	0.121
Total Mono-OH	0.000	0.001	0.000	0.000	0.000	0.066	0.008	0.900	0.003	0.001
Total Di-OH	0.000	0.000	0.000	0.000	0.000	0.002	0.002	0.644	0.000	0.000
Total Tri-OH	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.533	0.000	0.000
% Mono-OH	0.000	0.001	0.051	0.003	0.000	0.049	0.996	0.768	0.046	0.000
% Di-OH	0.200	0.351	0.207	0.384	0.078	0.721	0.094	0.156	0.448	0.948
% Tri-OH	0.003	0.012	0.761	0.175	0.019	0.221	0.879	0.148	0.109	0.003
Total 12 α -OH	0.000	0.000	0.000	0.000	0.000	0.047	0.135	0.778	0.002	0.000
Total non-12 α -OH	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.605	0.000	0.000
12 α -OH/ non12 α -OH	0.194	0.271	0.002	0.017	0.000	0.003	0.001	0.102	0.237	0.000
CA/ CDCA	0.000	0.000	0.423	0.709	0.733	0.074	0.039	0.456	0.008	0.749
% 12 α -OH	0.039	0.511	0.000	0.001	0.000	0.000	0.000	0.085	0.142	0.000
% non-12 α -OH	0.039	0.511	0.000	0.001	0.000	0.000	0.000	0.085	0.142	0.000
Total Primary	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.592	0.000	0.000
Total Secondary	0.000	0.000	0.030	0.118	0.000	0.309	0.111	0.747	0.101	0.221
Primary/ Secondary	0.014	0.355	0.000	0.002	0.000	0.000	0.000	0.993	0.005	0.000
% Primary	0.000	0.063	0.000	0.000	0.000	0.000	0.001	0.218	0.000	0.000
%Secondary	0.000	0.063	0.000	0.000	0.000	0.000	0.001	0.218	0.000	0.000