

Table S1. Sensitivity, linearity, accuracy, and precision of bile acids by ultra-high-performance liquid chromatography coupled with quadrupole-time-of-flight mass spectrometer analysis.

Compounds	Linear Formula	LOD ¹ (µg/kg)	LOQ ² (µg/kg)	Precision (%)		Accuracy (%)		
				CV ³ _{Intra}	CV _{Inter}	Low	Medium	High
norDCA	y = 0.651386 x + 8.381732E-004	0.03	0.09	1.19	2.88	102.43	100.37	97.93
DHCA	y = 0.450615 x - 7.223210E-005	0.06	0.19	5.66	1.60	97.65	100.81	100.18
7,12-diketoLCA	y = 0.331379 x + 2.739396E-004	0.08	0.27	0.42	2.17	101.59	102.81	98.81
6,7-diketoLCA	y = 0.502384 x + 6.877313E-004	0.08	0.28	0.19	5.00	98.05	101.30	99.61
3-ketoLCA	y = 0.323258 x - 0.004134	0.15	0.50	1.54	0.21	99.60	100.38	100.83
7-ketoLCA	y = 1.533500 x + 0.003542	0.03	0.11	0.77	8.37	104.91	101.85	98.66
12-ketoLCA	y = 0.499284 x + 2.390257E-004	0.02	0.12	1.17	2.37	103.55	98.55	101.05
7-DHCA	y = 0.388852 x - 0.001835	0.03	0.24	2.96	0.19	103.51	99.64	99.57
3-DHCA	y = 0.662617 x + 0.001249	0.07	0.08	4.51	4.10	94.89	111.04	101.55
apoCA	y = 0.277331 x + 1.573897E-004	0.09	0.30	8.10	1.09	115.55	106.22	106.25
isoLCA	y = 0.784308 x + 0.001987	0.05	0.18	8.87	6.42	93.08	101.21	100.82
isoalloLCA	y = 1.182057 x + 7.166959E-004	0.03	0.10	1.51	3.94	99.60	100.75	100.87
alloCA	y = 3.528376 x + 6.996823E-004	0.02	0.06	1.60	0.92	99.17	95.71	97.69
UCA	y = 6.058174 x + 0.003005	0.01	0.03	3.04	6.81	99.09	97.29	102.48
LCA	y = 1.009131 x + 0.030949	0.02	0.05	2.67	0.24	100.53	102.29	98.02
UDCA	y = 1.734014 x + 0.001762	0.05	0.16	1.78	5.20	105.58	101.29	100.08
CDCA	y = 1.412708 x + 9.372573E-004	0.04	0.12	6.71	3.73	98.59	96.06	100.39
isoDCA	y = 1.226037 x + 0.001227	0.02	0.07	6.23	5.15	101.08	100.86	99.49
MDCA	y = 0.837269 x + 2.348623E-004	0.03	0.11	0.97	1.86	103.05	100.81	99.76
DCA	y = 0.778721 x + 0.007314	0.02	0.08	4.22	7.39	97.86	102.05	100.93
HDCA	y = 0.465608 x - 3.247209E-004	0.06	0.21	4.45	5.48	107.44	98.12	95.47
α-MCA	y = 1.191828 x + 0.001271	0.04	0.13	5.23	3.81	101.62	102.24	102.53
β-MCA	y = 1.216027 x + 0.002118	0.03	0.10	4.21	8.35	107.83	105.21	103.69
γ -MCA	y = 1.401082 x + 7.317450E-004	0.03	0.10	0.17	6.19	103.39	100.25	99.87
ω-MCA	y = 1.470009 x + 0.023447	0.02	0.08	8.70	5.28	98.13	102.35	101.86
CA	y = 1.457358 x + 0.006402	0.02	0.08	9.78	0.79	106.04	103.18	105.02
GDHCA	y = 0.658480 x - 0.013658	0.04	0.14	5.70	1.76	105.33	96.20	98.54
GLCA	y = 1.120251 x - 0.004391	0.03	0.09	0.40	7.26	105.12	98.30	99.81
GDCA	y = 1.211294 x + 0.001554	0.04	0.14	3.65	2.47	99.37	102.33	98.36
GCDCA	y = 1.229572 x + 5.999672E-004	0.03	0.11	4.10	0.12	97.94	101.00	102.82
GUDCA	y = 1.561018 x - 0.015192	0.04	0.14	7.29	7.83	103.11	100.25	98.59
GHCA	y = 1.134934 x - 0.036098	0.04	0.10	0.04	5.29	100.99	104.23	100.11
GHDCA	y = 0.825538 x + 5.799325E-004	0.03	0.14	6.34	2.07	106.42	95.12	97.70
GCA	y = 0.795128 x + 0.006782	0.03	0.11	7.42	2.27	102.50	96.89	103.62
TLCA	y = 1.702910 x + 0.001291	0.03	0.10	6.94	0.34	100.89	102.46	98.92

TCDCA	$y = 1.156731 x + 0.004892$	0.03	0.10	7.74	3.98	103.56	102.80	99.13
TDCA	$y = 1.831847 x + 5.272285E-004$	0.03	0.09	4.52	7.77	109.69	106.03	99.15
TUDCA	$y = 1.079787 x + 0.006024$	0.03	0.11	8.77	0.29	102.36	103.64	100.50
THDCA	$y = 1.353724 x - 8.004187E-004$	0.04	0.12	9.05	4.74	96.30	100.09	98.42
T-β-MCA	$y = 1.844287 x + 0.003743$	0.03	0.11	2.52	4.30	106.81	101.75	94.90
THCA	$y = 1.788719 x - 0.009246$	0.04	0.12	1.46	2.24	100.32	99.87	102.19
TCA	$y = 1.396524 x + 7.956564E-004$	0.06	0.19	5.40	8.22	100.53	99.69	99.69
T-α-MCA	$y = 0.165350 x - 0.002958$	0.14	0.47	8.10	0.52	99.87	100.42	98.87
LCA-3S	$y = 1.498371 x + 0.013112$	0.04	0.13	1.70	3.54	101.84	101.87	96.22
UDCA-3S	$y = 1.576279 x + 0.004861$	0.03	0.10	8.42	7.30	106.03	99.74	94.89
CDCA-3S	$y = 1.249296 x + 0.004990$	0.03	0.11	5.17	9.98	104.81	100.90	94.88
DCA-3S	$y = 1.493935 x + 0.020683$	0.03	0.09	1.46	4.57	105.67	102.07	96.71
CA-3S	$y = 1.087670 x + 0.012822$	0.05	0.18	5.61	4.66	101.67	103.65	96.09
GLCA-3S	$y = 1.009221 x - 0.031716$	0.13	0.43	0.56	3.43	105.02	97.16	98.80
GUDCA-3S	$y = 0.998073 x - 0.007271$	0.09	0.31	0.94	5.98	99.75	97.86	103.65
GCDCA-3S	$y = 1.023463 x - 0.009598$	0.10	0.33	3.83	5.28	96.68	90.53	102.19
GDCA-3S	$y = 1.126820 x - 0.007818$	0.08	0.27	1.43	4.36	104.50	89.14	104.63
GCA-3S	$y = 1.032762 x - 0.003273$	0.09	0.30	3.50	3.41	103.65	96.96	102.96
TLCA-3S	$y = 1.319584 x - 0.004526$	0.24	0.81	3.77	6.93	92.39	98.99	102.89
TUDCA-3S	$y = 1.179070 x + 0.013669$	0.08	0.27	3.62	8.73	101.91	103.05	99.66
TCDCA-3S	$y = 1.213847 x + 0.003391$	0.11	0.38	6.33	6.90	106.13	101.90	99.74
TDCA-3S	$y = 1.267394 x + 0.007063$	0.11	0.38	6.64	5.21	105.06	98.60	100.89
TCA-3S	$y = 1.470925 x - 0.003398$	0.08	0.26	2.36	1.60	100.81	102.26	98.44

1 LOD—limits of detection
2 LOQ—limits of quantification
3 CV—coefficient variations

Table S2. The recovery (%) of spiked concentration (µg/kg) for bile acids in each biological sample.

Compounds	Rat							Mouse							Human						
	2.5	25	50	250	500	2500	5000	2.5	25	50	250	500	2500	5000	2.5	25	50	250	500	2500	5000
norDCA	108.93	98.95	103.89					95.62	98.32	108.42					117.38	99.75	114.25				
DHCA	106.45	93.30	104.49					108.60	95.66	107.40					104.09	101.03	109.96				
7,12-diketoLCA	105.32	98.94	104.44					80.22	96.39	113.56					115.34	117.31	113.22				
6,7-diketoLCA	107.60	100.34	99.31					111.32	104.95	108.73					91.53	96.54	93.37				
3-ketoLCA	109.49	95.25	111.95	96.99	105.44			105.09	120.83	92.17	102.69	102.72			103.36	93.20	103.96	99.50	99.34		
7-ketoLCA	108.67	100.99	103.38					101.14	95.60	106.35					91.37	94.95	92.28	107.10	90.19	102.69	
12-ketoLCA	96.16	94.99	104.87					84.15	97.43	108.32					108.09	88.94	98.27	101.24	85.19	105.99	
7-DHCA	102.83	101.38	98.57	112.46	103.06	118.65	112.15	106.73	98.78	103.67	100.72	98.19	113.58	105.47	100.08	96.83	102.04	117.78	103.25	93.49	
3-DHCA	83.91	93.46	102.33	106.02	104.21	116.63	112.08	117.78	97.35	107.59	99.19	100.21	118.65	101.61	110.44	81.12	81.47	119.34	88.96	108.54	
apoCA	82.78	103.70	83.56					103.47	112.19	95.53					89.11	101.45	116.95				
isoLCA	118.96	118.09	103.78					107.27	116.27	114.47					106.11	96.94	90.73				
isoalloLCA	105.75	100.52	92.81					115.82	97.12	99.27					102.83	105.38	97.98				
alloCA	85.43	99.16	85.91	114.53	91.63			92.20	108.41	111.19	101.31	99.29			96.62	101.55	105.96	107.96	101.40	97.92	99.76
UCA	89.89	106.97	105.43					118.79	99.31	111.07					80.32	97.13	88.24	112.51	103.96	105.46	95.74
LCA	102.16	101.33	102.93					111.59	100.05	108.75					120.54	110.19	94.90	92.65	91.33	107.08	98.76
UDCA	104.86	98.88	102.52					97.47	101.07	107.68					100.86	94.35	113.38				
CDCA	104.47	96.25	104.05					103.76	98.98	110.07					109.18	98.64	114.80				
isoDCA	95.85	89.39	106.39	100.65	110.58	116.20	108.58	103.53	115.65	114.97	103.85	98.21	115.11	103.60	117.01	103.51	113.38	109.79	93.17	103.99	98.86
MDCA	100.51	100.29	103.08	113.84	104.90			118.66	110.12	108.81	101.08	100.48			100.26	95.51	117.93				
DCA	84.71	97.77	107.68	115.66	107.24	119.46	112.41	114.08	107.18	107.97	102.41	105.82	117.89	105.66	102.85	103.08	112.28				
HDCA	106.98	98.06	105.57	109.30	110.95	117.13	110.58	92.94	109.84	114.59	103.77	103.68	112.66	106.18	103.35	103.97	115.97				
α-MCA	100.38	89.59	105.87	111.06	105.85			101.93	94.75	108.09	100.22	99.70			106.84	106.76	102.24				
β-MCA	107.78	100.14	102.90					98.65	99.66	110.74					83.10	96.29	113.67				
γ-MCA	106.06	94.96	102.35	110.70	108.10	112.54	114.09	116.00	99.54	109.22	101.76	102.66	120.66	112.06	111.24	88.71	81.04				
ω-MCA	87.55	82.30	88.17	110.97	110.55	119.39	111.53	103.17	96.74	120.81	115.12	107.02	114.09	104.28	83.89	82.72	88.64				
CA	89.27	87.11	104.60	106.38	104.31	116.47	110.75	114.11	99.06	113.95	98.84	102.08	114.93	104.97	95.46	101.39	109.69	107.12	92.82	111.46	93.19
GDHCA	99.10	98.85	101.05					98.52	96.94	104.17					117.01	94.26	115.08				
GLCA	116.43	92.61	100.06					106.31	100.19	106.21					103.52	113.01	112.42				
GDCA	103.43	95.95	104.67					100.55	100.95	108.50					95.07	82.07	107.51				
GCDCA	96.98	99.61	105.70					96.08	106.42	101.87					92.38	82.80	101.08				

GUDCA	104.59	104.01	100.31			91.86	102.93	107.10			99.92	89.11	112.78			
GHCA	116.61	112.44	101.24			91.01	92.10	103.58			83.57	96.55	99.38			
GHDCA	92.70	100.80	95.95			99.55	101.06	101.70			91.17	101.62	95.60			
GCA	112.35	96.92	100.23			112.10	95.55	105.24			101.02	80.22	97.25			
TLCA	104.41	99.80	105.69			107.70	106.15	108.33			93.36	94.86	96.45			
TCDCA	84.92	79.48	106.24	111.38	109.27	108.71	98.76	104.64	99.13	99.94	90.01	94.47	117.19			
TDCA	103.01	96.07	103.01			100.95	98.56	109.96			118.39	93.51	109.90			
TUDCA	94.05	99.52	105.89	113.31	109.21	93.23	97.49	110.76	98.39	103.61	99.61	94.21	110.88			
THDCA	80.99	97.25	98.44			106.09	103.96	113.75			103.00	100.26	90.43			
T-β-MCA	104.58	104.04	104.98			108.01	99.18	100.66			114.29	94.37	106.81			
THCA	108.89	100.01	101.60	106.16	102.87	110.06	98.16	107.81	96.89	101.00	113.68	100.16	105.41			
TCA	98.79	84.76	101.35	113.31	108.69	115.81	102.32	101.97	100.23	101.30	108.38	108.91	103.64			
T-α-MCA	109.73	92.74	101.63	113.40	105.93	111.59	111.65	108.61	95.11	104.64	93.19	100.69	102.31			
LCA-3S	107.02	100.85	102.12			116.46	98.19	109.57			100.72	99.32	107.15	105.06	99.94	96.84
UDCA-3S	105.72	102.82	101.10			109.37	98.22	105.57			105.42	103.83	102.86	113.08	94.47	97.95
CDCA-3S	91.62	82.47	106.11			104.91	100.64	106.20			104.74	97.23	105.98	99.76	98.56	106.68
DCA-3S	100.58	107.63	103.78			102.95	103.27	110.31			102.45	100.71	99.22	96.52	95.40	96.22
CA-3S	103.55	100.24	101.82			102.98	99.45	110.11			95.63	93.15	101.66	101.01	98.22	93.07
GLCA-3S	103.87	101.66	100.61			119.15	95.38	105.20			99.28	107.88	107.87			
GUDCA-3S	131.94	101.37	98.71			93.86	106.90	101.82			91.49	100.12	102.43			
GCDCA-3S	126.66	87.54	101.78			118.40	85.21	106.49			95.41	96.92	99.84			
GDCA-3S	110.11	105.98	102.97			101.12	80.47	111.00			109.73	108.99	98.78			
GCA-3S	100.63	93.83	100.55			98.16	98.22	110.66			99.69	98.49	98.69			
TLCA-3S	94.28	96.48	107.01			116.77	94.55	109.38			95.96	99.83	97.12			
TUDCA-3S	103.54	107.48	105.78			82.02	100.25	110.41			99.54	96.67	96.96			
TCDCA-3S	100.54	102.85	117.10			111.10	97.64	116.98			102.43	102.52	105.02			
TDCA-3S	105.13	97.12	105.54			106.01	102.31	106.75			90.88	106.23	95.52			
TCA-3S	82.46	80.50	104.88	100.00	104.34	94.02	100.17	108.18	98.95	96.16	101.88	100.33	94.27			

Table S3. The matrix effect (%) of spiked concentration (µg/kg) for bile acids in each biological sample.

Compounds	Rat							Mouse							Human						
	2.5	25	50	250	500	2500	5000	2.5	25	50	250	500	2500	5000	2.5	25	50	250	500	2500	5000
norDCA	103.64	103.78	105.84					100.12	100.86	104.21					106.60	110.34	104.33				
DHCA	93.94	87.11	116.66					98.96	88.91	108.14					122.12	102.26	106.37				
7,12-diketoLCA	91.32	97.97	106.96					99.26	102.07	103.04					88.31	104.22	92.00				
6,7-diketoLCA	96.27	103.03	103.95					101.99	99.52	104.57					112.40	109.81	117.02				
3-ketoLCA	106.04	91.73	96.96	98.09	87.49			102.79	100.89	64.23	103.54	98.76			110.22	108.57	108.20	95.58	111.27		
7-ketoLCA	103.66	99.17	103.12					109.42	98.78	106.04					111.81	84.51	111.48	95.17	109.48	101.08	
12-ketoLCA	81.31	104.61	105.21					83.71	86.09	103.14					90.35	110.12	97.09	98.64	108.33	99.20	
7-DHCA	111.20	100.23	108.85	98.61	106.30	99.73	98.99	100.67	108.65	111.19	105.45	110.95	108.98	106.87	114.66	99.65	81.16	113.40	109.02	98.46	
3-DHCA	112.18	102.51	110.86	100.06	103.92	103.71	97.70	103.07	108.02	109.01	103.23	105.76	119.53	106.34	98.70	103.06	100.45	84.13	100.74	102.93	
apoCA	80.05	84.93	88.55					118.15	106.44	82.78					101.69	87.51	85.88				
isoLCA	97.35	101.62	88.08					86.69	90.56	94.17					93.35	96.92	108.08				
isoalloLCA	110.62	91.47	116.74					102.35	121.56	123.14					88.52	107.91	99.12				
alloCA	85.47	89.60	97.52	93.66	107.70			136.48	110.46	104.35	104.56	103.56			88.90	97.59	98.54	87.14	112.83	103.46	99.76
UCA	112.65	93.69	105.91					108.59	110.97	103.22					106.70	94.33	117.13	85.47	105.51	100.77	95.74
LCA	111.51	99.79	103.52					116.20	106.94	100.95					93.68	103.20	85.70	82.84	84.05	99.24	98.76
UDCA	98.71	103.13	103.27					98.62	93.56	105.01					120.16	110.22	99.87				
CDCA	104.70	104.60	104.78					108.56	94.32	106.75					118.74	98.06	94.76				
isoDCA	86.67	80.52	111.21	98.59	106.61	103.49	98.39	85.98	108.14	107.53	97.45	99.05	104.67	102.45	96.17	98.63	86.95	88.74	112.58	100.71	98.86
MDCA	100.84	107.69	104.87	98.03	104.76			104.66	108.00	102.76	87.54	90.54			102.82	99.89	93.85				
DCA	102.28	109.14	107.70	94.23	108.38	102.31	98.48	93.76	106.63	105.57	98.65	103.56	98.67	102.46	120.91	106.77	99.30				
HDCA	108.15	118.81	119.66	106.74	113.54	103.35	99.01	114.90	106.89	91.68	109.54	96.55	98.03	104.62	96.13	102.93	107.84				
α-MCA	113.32	99.28	103.60	95.84	106.95			103.37	107.73	102.33	98.34	90.35			81.99	97.85	96.93				
β-MCA	101.87	98.80	103.73					106.37	104.64	103.22					105.16	97.27	84.06				
γ -MCA	98.74	105.25	102.81	97.95	107.11	108.19	94.92	95.26	105.42	104.67	109.45	114.32	116.34	98.54	97.58	93.40	95.86				
ω-MCA	115.54	100.05	103.05	96.43	104.70	101.58	97.45	80.52	106.21	97.96	115.12	107.02	114.09	104.28	86.78	94.58	99.42				
CA	82.90	94.05	100.53	95.16	111.00	100.85	98.06	96.34	108.79	100.02	99.34	105.34	116.32	102.54	100.67	96.07	86.83	84.34	95.94	95.00	93.19
GDHCA	118.86	100.97	110.45					120.45	114.76	111.14					93.98	114.29	101.06				
GLCA	94.11	105.61	101.21					97.74	103.76	101.34					103.61	99.15	98.53				
GDCA	106.22	104.28	106.27					109.05	108.68	105.12					98.31	104.81	95.33				

GCDCA	113.80	104.66	107.38			113.70	109.54	106.67			106.92	84.38	95.62			
GUDCA	101.15	101.65	99.01			107.85	109.76	104.21			113.83	115.14	100.32			
GHCA	103.57	89.27	107.23			104.83	108.97	110.87			102.84	106.82	98.79			
GHDCA	100.44	100.36	104.76			116.52	112.23	113.14			95.36	84.64	94.25			
GCA	100.69	98.77	99.62			102.52	104.56	106.23			111.09	108.15	96.92			
TLCA	112.53	104.50	103.15			119.88	110.67	98.95			80.47	108.44	97.01			
TCDCa	102.38	99.12	103.38	95.96	103.87	110.74	105.12	106.35	90.32	93.21	118.54	107.28	96.36			
TDCA	98.54	101.32	104.38			109.18	106.76	105.07			85.80	106.00	97.19			
TUDCA	106.83	99.23	101.01	94.41	107.80	115.95	106.31	99.85	109.32	112.45	96.42	105.63	97.93			
THDCA	85.03	106.05	102.47			90.54	97.56	98.41			97.25	95.06	101.89			
T-β-MCA	118.82	99.16	100.10			103.39	99.05	105.76			103.37	106.70	112.66			
THCA	102.35	100.63	105.38	98.28	113.40	100.29	113.01	104.82	90.34	87.40	94.65	112.25	96.44			
TCA	93.15	101.76	105.94	96.46	103.30	101.77	105.81	108.59	98.03	104.34	87.46	92.82	87.62			
T-α-MCA	85.51	105.71	103.22	91.50	107.00	105.98	106.89	105.19	98.45	113.23	93.16	102.62	97.05			
LCA-3S	103.60	99.50	103.02			104.27	98.67	102.96			90.52	81.51	91.30	82.15	109.05	106.98
UDCA-3S	98.72	100.63	101.78			91.20	100.53	103.56			96.40	111.78	114.95	103.41	111.58	106.15
CDCA-3S	94.91	98.95	108.90			107.70	103.24	107.32			93.90	81.48	83.07	93.99	108.52	92.73
DCA-3S	103.57	99.37	102.65			95.27	116.56	105.66			83.30	95.92	99.28	101.33	108.28	104.62
CA-3S	108.69	101.88	97.03			108.23	107.68	98.81			114.26	97.42	99.91	96.65	108.77	102.69
GLCA-3S	113.67	99.43	99.10			88.49	104.64	99.84			94.24	110.79	100.70			
GUDCA-3S	85.62	102.96	105.81			102.24	103.56	111.77			93.02	107.99	100.14			
GCDCA-3S	94.39	97.12	108.16			105.45	98.65	113.25			101.22	119.14	117.18			
GDCA-3S	103.49	81.38	106.18			112.74	102.67	107.66			102.10	103.09	106.40			
GCA-3S	106.23	101.88	107.32			101.94	102.45	110.02			110.93	87.51	100.63			
TLCA-3S	105.10	100.97	112.20			94.09	98.75	110.07			97.21	101.55	115.57			
TUDCA-3S	107.09	98.31	106.81			108.58	97.53	103.99			90.34	105.28	107.20			
TCDCa-3S	106.44	92.27	95.13			98.76	97.42	91.30			102.26	119.02	112.44			
TDCA-3S	111.60	107.33	104.44			86.47	114.52	106.93			96.88	91.18	94.10			
TCA-3S	92.96	98.99	110.03	99.64	103.26	105.66	107.82	103.74	98.95	96.16	102.03	89.90	99.75			