Supplemental Table S1. Typical MRM ion pairs for establishment of comprehensive profile of urinary bile acids in piglets

Forms of conjugates	Negative ion mode							
	TetraOH BA	TriOH BA	DiOH BA	MonoOH BA	TriOH BA-Δ^4-3-one	DiOH BA-Δ^4-3-one	MonoOH BA-Δ^4-3-one	BA-Δ^4-3-one
Free BAs	423.4[1] 423.4/405.3	407.4[1] 407.4/343.2 407.4/389.4	391.4[1] 391.4/373.2 391.4/345.5	375.4[1] 375.4/357.2	419.4[1]	403.4[1] 403.4/123.1	387.4[1] 387.4/369.4	371.4[1]
T-BAs	530.6/124.0	514.6/124.0	498.6/124.0	482.6/124.0	526.6/124.0	510.6/124.0	494.6/124.0	478.6/124.0
G-BAs	480.6/74.0	464.6/74.0	448.6/74.0	432.6/74.0	476.6/74.0	460.6/74.0	444.6/74.0	428.6/74.0
BA-S	503.6/97.0	487.6/97.0	471.6/97.0	455.6/97.0	499.6/97.0	483.6/97.0	467.6/97.0	
T-BA-S	304.9[2]/97.0 610.8/97.0 610.8/124.0	296.9[2]/97.0 594.8/97.0 594.8/124.0	288.9[2]/97.0 578.8/97.0 578.8/124.0	280.9[2]/97.0 562.8/97.0 562.8/124.0	302.9[2]/97.0 606.7/97.0 606.7/124.0	294.9[2]/97.0 590.7/97.0 590.7/124.0	286.9[2]/97.0 574.7/97.0 574.7/124.0	
G-BA-S	279.8[2]/97.0 560.7/97.0 560.7/74.0	271.8[2]/97.0 544.7/97.0 544.7/74.0	263.8[2]/97.0 528.7/97.0 528.7/74.0	255.8[2]/97.0 512.7/97.0 512.7/74.0	277.8[2]/97.0 556.7/97.0 556.7/74.0	269.8[2]/97.0 540.7/97.0 540.7/74.0	261.8[2]/97.0 524.7/97.0 524.7/74.0	
BA-GlcUA	599.7/423.4	583.7/407.4	567.7/391.4	551.7/375.4	595.7/419.4	579.7/403.4	563.7/387.4	
T-BA-GlcUA	706.8/124.0 706.8/423.4	690.8/124.0 690.8/407.4	674.8/124.0 674.8/391.4	658.8/124.0 658.8/375.4	702.8/124.0 702.8/419.4	686.8/124.0 686.8/403.4	670.8/124.0 670.8/387.4	
G-BA-GlcUA	656.7/74.0 656.7/423.4	640.7/74.0 640.7/407.4	624.7/74.0 624.7/391.4	608.7/74.0 608.7/375.4	652.7/74.0 652.7/419.4	636.7/74.0 636.7/403.4	620.7/74.0 620.7/387.4	
BA-GlcNAc	626.8/423.4	610.8/407.4	594.8/391.4	578.8/375.4	622.7/419.4	606.7/403.4	590.7/387.4	
T-BA-GlcNAc	733.9/124.0 733.9/423.4	717.9/124.0 717.9/407.4	701.9/124.0 701.9/391.4	685.9/124.0 685.9/375.4	729.9/124.0 729.9/419.4	713.9/124.0 713.9/403.4	697.9/124.0 697.9/387.4	
G-BA-GlcNAc	683.8/74.0 683.8/423.4	667.8/74.0 667.8/407.4	651.8/74.0 651.8/391.4	635.8/74.0 635.8/375.4	679.8/74.0 679.8/419.4	663.8/74.0 663.8/403.4	647.8/74.0 647.8/387.4	
BA-GlcA	585.7/423.4	569.7/407.4	553.7/391.2	537.7/375.4	581.7/419.4	565.7/403.4	549.7/387.4	
T-BA-GlcA	692.8/124.0 692.8/423.4	676.8/124.0 676.8/407.4	660.8/124.0 660.8/391.4	644.8/124.0 644.8/375.4	688.8/124.0 688.8/419.4	672.8/124.0 672.8/403.4	656.8/124.0 656.8/387.4	

G-BA-GlcA	642.7/74.0 642.7/423.4	626.7/74.0 626.7/407.4	610.7/74.0 610.7/391.4	594.7/74.0 594.7/375.4	638.7/74.0 638.7/419.4	622.7/74.0 622.7/403.4	606.7/74.0 606.7/387.4
BA-S-GlcUA	679.8/423.4 679.8/97.0	663.8/407.4 663.8/97.0	647.8/391.4 647.8/97.0		675.7/419.4 675.7/97.0	659.7/403.4 659.7/97.0	
T-BA-S-GlcUA	392.9[2]/97.0 786.8/124.0 786.8/97.0	384.9[2]/97.0 770.8/124.0 770.8/97.0	376.9[2]/97.0 754.8/124.0 754.8/97.0		390.9[2]/97.0 782.8/124.0 782.8/97.0	382.9[2]/97.0 766.8/124.0 766.8/97.0	
G-BA-S-GlcUA	367.9[2]/97.0 736.8/74.0 736.8/97.0	359.9[2]/97.0 720.8/74.0 720.8/97.0	351.9[2]/97.0 704.8/74.0 704.8/97.0		365.9[2]/97.0 732.7/74.0 732.7/97.0	357.8[2]/97.0 716.7/74.0 716.7/97.0	
BA-S-GlcNAc	706.8/423.4 706.8/97.0	690.8/407.4 690.8/97.0	674.8/391.4 674.8/97.0		702.8/419.4 702.8/97.0	686.8/403.4 686.8/97.0	
T-BA-S-GlcNAc	406.4[2]/97.0 813.9/124.0 813.9/97.0	398.4[2]/97.0 797.9/124.0 797.9/97.0	390.4[2]/97.0 781.9/124.0 781.9/97.0		404.4[2]/97.0 809.8/124.0 809.8/97.0	396.4[2]/97.0 793.9/124.0 793.9/97.0	
G-BA-S-GlcNAc	381.4[2]/97.0 763.8/74.0 763.8/97.0	373.4[2]/97.0 747.8/74.0 747.8/97.0	365.4[2]/97.0 731.8/74.0 731.8/97.0		379.4[2]/97.0 759.8/74.0 759.8/97.0	371.4[2]/97.0 743.8/74.0 743.8/97.0	
BA-S-GlcA	665.8/423.4 665.8/97.0	649.8/407.4 649.8/97.0	633.8/391.4 633.8/97.0		661.7/419.4 661.7/97.0	645.7/403.4 645.7/97.0	
T-BA-S-GlcA	385.9[2]/97.0 772.9/124.0 772.9/97.0	377.9[2]/97.0 756.9/124.0 756.9/97.0	369.9[2]/97.0 740.9/124.0 740.9/97.0		383.9[2]/97.0 768.8/124.0 768.8/97.0	375.9[2]/97.0 752.8/124.0 752.8/97.0	
G-BA-S-GlcA	360.9[2]/97.0 722.8/74.0 722.8/97.0	352.9[2]/97.0 706.8/74.0 706.8/97.0	344.9[2]/97.0 690.8/74.0 690.8/97.0		358.9[2]/97.0 718.8/74.0 718.8/97.0	350.9[2]/97.0 702.8/74.0 702.8/97.0	

[1] A selected ion $[M-H]^-$ was used to monitor unconjugated BAs.

[2] The ion is doubly charged ion, $[M-2H]^{2-}$.

Supplemental Table S2. Calibration curves and quantitation of urinary bile acids

No. in Table 1	Standards	Equation	Correlation Coefficient (R^2)	For quantitation of BAs (No. in Table 1)
5, S1	ωMCA	y = 406.68x - 0.3232	0.9999	1-6, 17-19, 52-57
7, S4	γMCA	y = 350.02x - 22.6950	0.9999	7
9, S7	T-βMCA	y = 24074x + 8.2243	0.9998	8-10
S8	T-γMCA	y = 16674x + 2.0412	0.9997	20-25, 20a, 25a, 58
16, S10	G-γMCA	y = 389.61x + 0.2528	1.000	11-16, 59-76,
26, S12	MDCA	y = 620.8x - 1.8310	0.9998	26
27, S14	HDCA	y = 612.73x - 2.4817	0.9998	27
28, S16	CDCA	y = 738.39x - 6.5608	0.9997	28
29, S17	DCA	y = 152.81x - 0.8603	1.000	29
32, S24	G-HDCA	y = 281.58x - 0.9227	0.9999	30-32, 34-38, 40-42, 42a
33, S25	G-CDCA	y = 344.82x - 2.6177	0.9998	33,39
45, S28	CDCA-3S disodium salt	y = 372.69x - 2.9111	0.9998	43-51
77, S29	alloLCA	y = 1880.4x - 2.6415	0.9995	77
78, S31	LCA	y = 866.84x + 0.2139	1.0000	78
S32	T-LCA	y = 53306x - 36.9860	0.9998	82-86
S33	G-LCA	y = 336.31x - 3.6079	0.9999	79-80
S34	G-LCA-3S disodium salt	y = 4458.8x + 0.2940	0.9999	81