

Supplementary Table 3 Calibration curves of each analytes and matrix factor of analytes and IS.

(A) Standard calibration curves

No	Compound	Quantitation range (ng/mL)	Regression equation	Correlation coefficient
1	SNAG- $\Delta^5$ -CA	0.3–1000	$y=0.00725x+0.0000317$	0.998
2	SNAG- $\Delta^5$ -CG	0.3–1000	$y=0.00751x+0.000778$	0.999
3	SNAG- $\Delta^5$ -CT	0.3–1000	$y=0.0111x+0.000224$	1.000
4	S7B- $\Delta^5$ -CA	0.3–1000	$y=0.00397x+0.000246$	0.997
5	S7O- $\Delta^5$ -CA	0.3–1000	$y=0.00847x+0.000216$	0.998

(B) Matrix factors

No	Compound	Matrix factor (%)	IS normalized matrix factor (%)
1	SNAG- $\Delta^5$ -CA	102	101
2	SNAG- $\Delta^5$ -CG	103	102
3	SNAG- $\Delta^5$ -CT	105	104
4	S7B- $\Delta^5$ -CA	102	101
5	S7O- $\Delta^5$ -CA	105	104
6	IS	101	-

N=3.

SNAG- $\Delta^5$ -CA, 3 $\beta$ -Sulfooxy-7 $\beta$ -*N*-acetylglucosaminyl-5-cholenoic acid; SNAG- $\Delta^5$ -CG, Glycine-amidated

3 $\beta$ -sulfooxy-7 $\beta$ -*N*-acetylglucosaminyl-5-cholenoic acid; SNAG- $\Delta^5$ -CT, Taurine-amidated

3 $\beta$ -sulfooxy-7 $\beta$ -*N*-acetylglucosaminyl-5-cholenoic acid; S7B- $\Delta^5$ -CA, 3 $\beta$ -Sulfooxy-7 $\beta$ -hydroxy-5-cholenoic acid; S7O- $\Delta^5$ -CA, 3 $\beta$ -Sulfooxy-7-oxo-5-cholenoic acid; IS, internal standard.