Supplementary Table 1 MS/MS parameters in selected reaction monitoring.

No	Compound	Q1 (*m/z*)	Q3 (*m/z*)	DP (V)	EP (V)	CE (V)	CXP (V)
1	SNAG-Δ^5-CA	672.3	97.0	-70	-8	-70	-14
2	SNAG-Δ^5-CG	364.2	97.0	-30	-10	-42	-14
3	SNAG-Δ^5-CT	389.2	97.0	-100	-14	-42	-14
4	S7B-Δ^5-CA	469.2	97.0	-320	-12	-80	-14
5	S7O-Δ^5-CA	467.1	97.0	-240	-12	-60	-14
6	IS	455.3	97.0	-80	-12	-75	-10

CE, Collision energy; CXP, Collision cell exit potential; DP, Declustering potential; EP, Entrance potential; SNAG-Δ^5-CA, 3β-Sulfooxy-7β-*N*-acetylglucosaminyl-5-cholenoic acid; SNAG-Δ^5-CG, Glycine-amidated 3β-sulfooxy-7β-*N*-acetylglucosaminyl-5-cholenoic acid; SNAG-Δ^5-CT, Taurine-amidated 3β-sulfooxy-7β-*N*-acetylglucosaminyl-5-cholenoic acid; S7B-Δ^5-CA, IS, internal standard, 3β-Sulfooxy-7β-hydroxy-23-*nor*-5-cholenoic acid; 3β-Sulfooxy-7β-hydroxy-5-cholenoic acid; S7O-Δ^5-CA, 3β-Sulfooxy-7-oxo-5-cholenoic acid; IS, internal standard.