## **Electronic supplementary information**

Figure S1



Fig. S1. Comparison of signal to noise ratios (SNRs) of several BAs at the lower limit of detection (LOD) in positive and negative ion modes.

Figure 2S



Fig. S2. Comparison of molecular ion intensity of LCA in negative ion mode (375.3  $\rightarrow$  375.3; *upper panel*) and positive ion mode (359.3  $\rightarrow$  135.1; *lower panel*) using MRM. The signal to noise ratio (SNR) of the latter was 4.0, thus above the lower limit of detection.

Bile acids	Extract recovery (%)
CA	$84 \pm 12$
CDCA	$79 \pm 20$
DCA	$67 \pm 19$
7-oxoDCA	$71 \pm 23$
HDCA	$80\pm 6$
LCA	$74 \pm 17$
7-oxoLCA	$76 \pm 13$
α-ΜCΑ	$72 \pm 15$
β-ΜCΑ	$70 \pm 11$
ω-MCA	$73 \pm 12$
UDCA	$79 \pm 11$
G-CA	$68 \pm 19$
G-CDCA	$69 \pm 17$
G-DCA	$76 \pm 24$
G-LCA	$75 \pm 11$
G-7-oxoLCA	$76 \pm 15$
G-UDCA	$76\pm16$
T-CA	$86 \pm 17$
T-CDCA	$80 \pm 17$
T-DCA	$88 \pm 10$
T-LCA	$82\pm9$
T-7-oxoLCA	$77 \pm 19$
Τ-β-ΜCΑ	$81 \pm 15$
T-UDCA	$74 \pm 23$

Data are presented as the average  $\pm$  % R.S.D of two levels of QC concentrations (200 nM and 2000 nM), six samples per concentration.