



Supplemental Figure 1. Extracted chromatograms for [M-H]⁻ ions, product ion MS/MS spectra and TLC separation for the major 15R-TIC metabolites.

(A) Ion chromatograms of deprotonated ions (m/z 355, 531, and 559) in human hepatocyte extracts incubated with 15R-TIC for 4 hours. (B) Product ion MS/MS spectra of the major metabolites of 15R-TIC. M1 is produced by de-ethylation of 15R-TIC, and M3 and M4 are glucuronide conjugates of 15R-TIC and M1, respectively. (C) Analysis of authentic 15R-TIC and metabolites (M1, M3 and M4) by TLC. M1, M3, and M4 were isolated by HPLC from rat bile samples and analyzed by TLC with phosphomolybdic acid staining. TLC analysis of each compound showing m/z 355, 559 and 531 ions observed by LC/MS produced major spots with retention factor (R_f) values of 0.35, 0.55, and 0.70, which corresponded to the expected R_f values for M1, M3 and M4, respectively.