



**Figure S3.** Chromatographic profile obtained by HPLC-ESI-MS/MS in positive ionization mode (left) or negative ionization mode (right) for light roast (panel A), dark roast (B), and decaffeinated coffee (C). The main compounds detected were caffeic acid (5.5 min), 3-*O*-caffeoylquinic acid (17.5 min), caffeine (20.5 min), 5-*O*-caffeoylquinic acid (21.8 min), 3-*O*-feruloylquinic acid (23.5 min) and 4-*O*-caffeoylquinic acid (26.0 min). The 5-*O*-feruloylquinic acid was not detected in positive ionization mode and caffeine was not detected in negative ionization mode.