

Figure S1. Phytochemical - target protein network (A), disease protein - protein (B) and a new phytochemical - target protein network (C). Phytochemicals and proteins were labeled as blue hexagon and green round, respectively.



Figure S2. UPLC-MS positive and negative total ion chromatogram of Rhubarb serum pharmacochemistry. Absorption components were labeled as digital: 1 Rhein, 2 Physcion, 3 Aloe-Emodin, 4 Emodin, 5 Physcionin, 6 Rhaponticin, 7 Catechin, 8 Epicatechin, 9 Chrysophanol, 10 Astringin.



Figure S3. A typical TIC chromatogram of urine in negative ESI mode.



Figure S4. Metabolite - protein network (A), extended pathway protein - protein network (B) and new metabolite - pathway protein network (C). Metabolite and pathway protein were labeled as purple square and red round, respectively. The interaction between protein and protein were linked by blue edge.



Figure S5. Absorption component – protein - metabolite network. Absorption component, disease protein, pathway protein and metabolite were labeled as blue hexagon, green round, red round and purple square, respectively.