

## Supporting Information

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

Figure S2. UPLC-MS positive and negative total ion chromatogram of rhubarb serum pharmacology. Absorbed 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. Component - protein - metabolite network. Component, disease protein, pathway protein and metabolite were labeled as blue hexagon, green round, red round and purple square, respectively.

Table S1. All selected genes from OMIM, GAD, TTD and DrugBank.

Table S2. 113 molecules collected from Comprehensive Natural Products in TCM and Reaxys databases.

Table S3. The information of the known targets, positive drugs and cutoff values.

Table S4. Identification Results of Potential Biomarkers by UPLC-Q-TOF.