Supporting Information

Renal Medulla is More Sensitive to Cisplatin than Cortex Revealed by Untargeted Mass Spectrometry-Based Metabolomics in Rats

Pei Zhang[1,2,3], Jia-Qing Chen[1,2,3], Wan-Qiu Huang[1,2,3], Wei Li[1,2,3], Yin Huang[1,2,3], Zun-Jian Zhang[1,2,3*] and Feng-Guo Xu[1,2,3*]

[1] Key Laboratory of Drug Quality Control and Pharmacovigilance (Ministry of Education), China Pharmaceutical University, Nanjing 210009, P. R. China.

[2] Jiangsu Key Laboratory of Drug Screening, China Pharmaceutical University, Nanjing 210009, P. R. China.

[3] State Key Laboratory of Natural Medicine, China Pharmaceutical University, Nanjing 210009, P. R. China.

* Corresponding author:

Feng-Guo Xu,

Key Laboratory of Drug Quality Control and Pharmacovigilance (China Pharmaceutical University),

Ministry of Education, Tongjiaxiang No. 24, Nanjing 210009, China;

Tel/Fax: +86 025 83271021; E-mail: fengguoxu@gmail.com

Zun-Jian Zhang,

Key Laboratory of Drug Quality Control and Pharmacovigilance (China Pharmaceutical University),

Ministry of Education, Tongjiaxiang No. 24, Nanjing 210009, China;

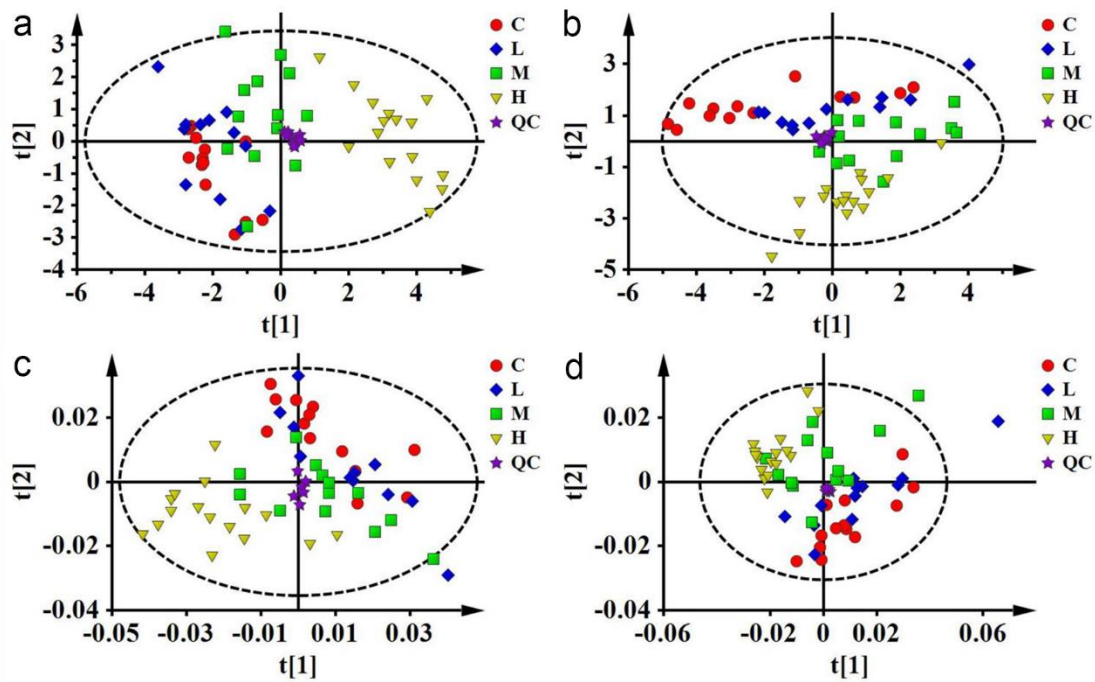Tel/Fax: +86 025 83271454; E-mail: zunjianzhangcpu@hotmail.com

Figure S1. Data quality evaluation for untargeted metabolomics using PCA. PCA score plot of (a) QCs and cortex samples based on GC-MS data, model parameter: $R^2X=0.48$, $Q^2=0.366$; (b) QCs and medulla samples based on GC-MS data, model parameter: $R^2X=0.671$, $Q^2=0.568$; (c) QCs and cortex samples based on LC-MS data, model parameter: $R^2X=0.593$, $Q^2=0.307$, and (d) QCs and medulla samples based on LC-MS data, model parameter: $R^2X=0.629$, $Q^2=0.297$.
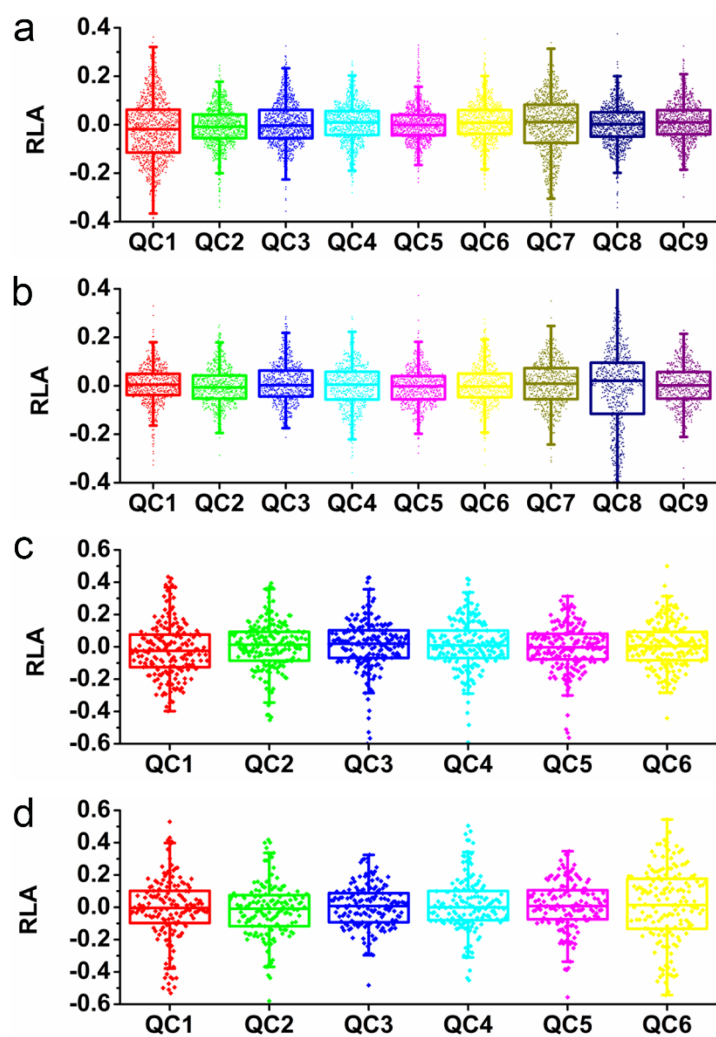
Figure S2. Data quality evaluation for untargeted metabolomics using RLA plot. RLA plot of (a) QCs of cortex in GC-MS analysis; (b) QCs of medulla in GC-MS analysis; (c) QCs of cortex in LC-MS analysis, and (d) QCs of medulla in LC-MS analysis.
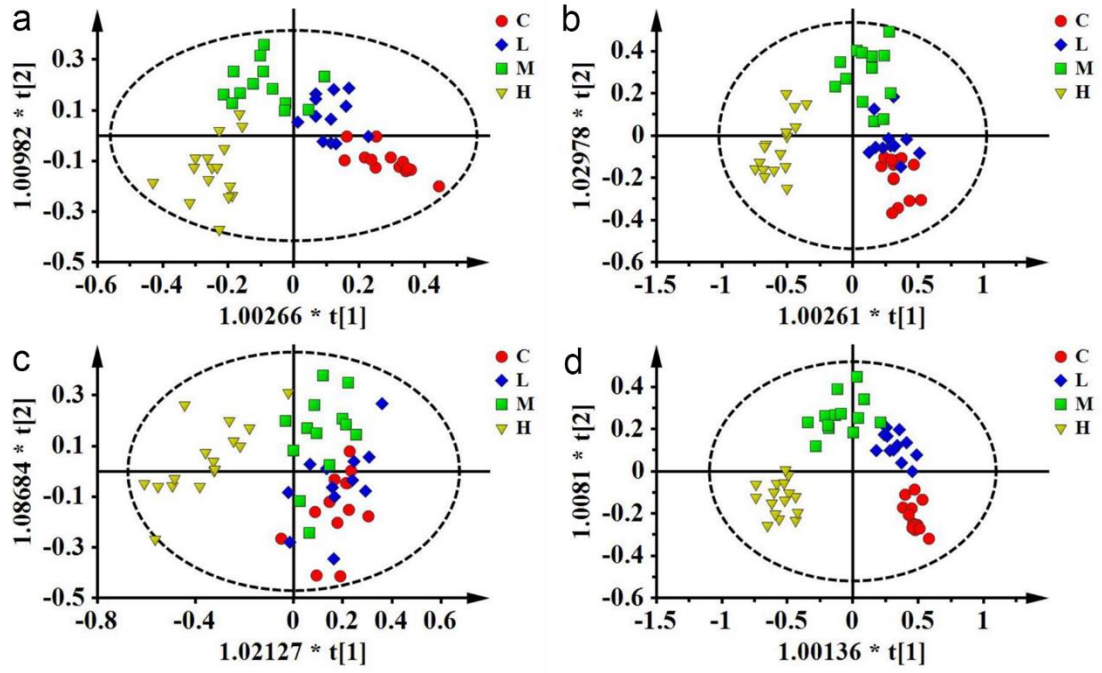
Figure S3. OPLS-DA score plots of (A) cortex samples based on GC-MS data; (B) cortex samples based on LC-MS data; (C) medulla samples based on GC-MS data and (D) medulla samples based on LC-MS data.
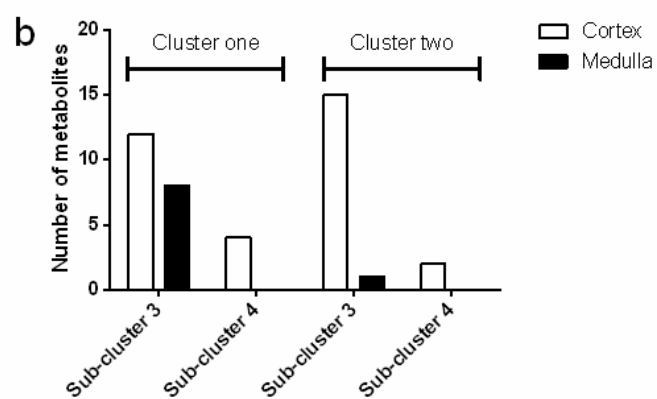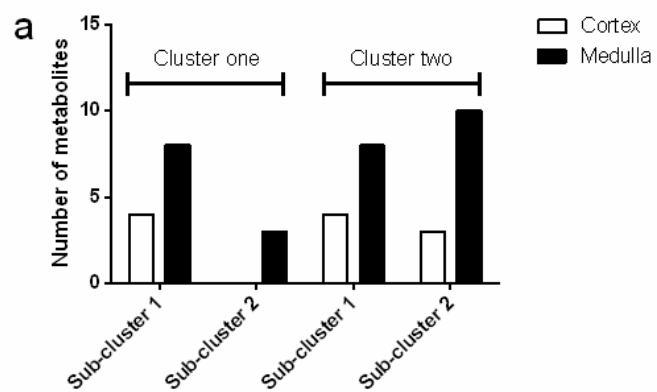
Figure S4 Histogram of the number of metabolites. (a) Metabolites in sub-cluster 1 and 2 withine cluster one and two; (b) Metabolites in sub-cluster 3 and 4 within cluster one and two.
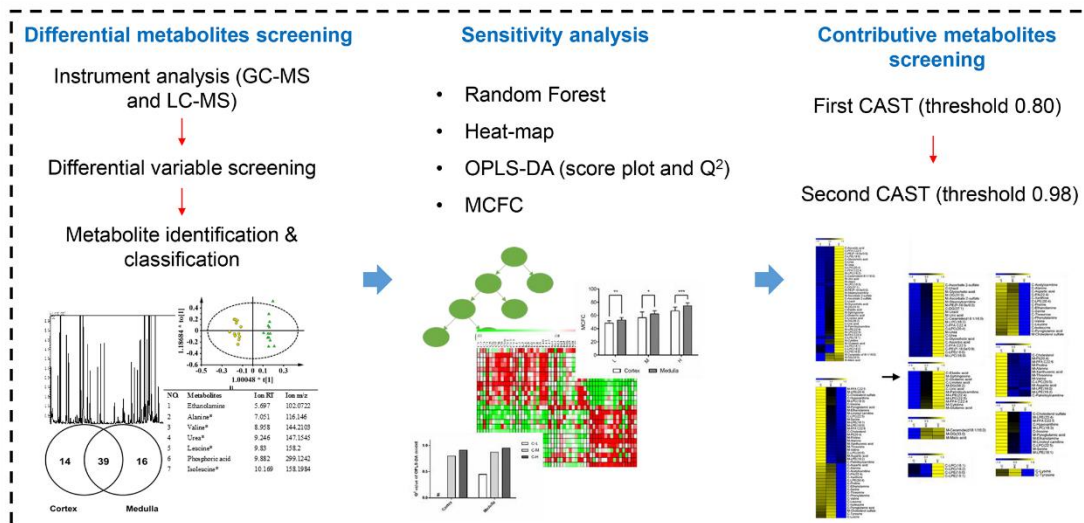
Figure S5. Strategy for differential metabolites screening, sensitivity analysis and contributory metabolites screening.