Supporting information: Supplementary Figures 1-7

Development of an Integrated Metabolomic Profiling Approach for

Infectious Diseases Research

Running title: Urinary Metabolomics to Infectious Diseases

By

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Supplemental Figure 1. Representative negative ion, LC/MS BPI chromatograms of a urine sample analyzed with different ion source voltages.

(A) -4000 V; (B) -4500 V



Supplemental Figure 2. Representative negative ion, LC/MS BPI chromatograms from a urine sample analyzed using increasing turbo source gun temperatures.

(A) 550°C; (B) 600°C; (C) 650°C



Supplemental Figure 3. Representative negative ion, LC/MS BPI chromatograms from a urine sample analyzed using increasing curtain gas (nitrogen) flows .

(A) 25 psi; (B) 35 psi



Supplemental Figure 4. Representative negative ion, LC/MS BPI chromatograms from a urine sample analyzed using increasing nebulizer gas (air) and turbo gas (air) flows.

(A) 50 psi; (B) 60 psi



Supplemental Figure 5. 3D Scatter score plot from PCA modeling of quality control analyses.



Supplemental Figure 6. Goodness of fit of modeling supports PLS_DA and OPLS_DA.

(A) The goodness of fit bar plot for R2Y (cum) and Q2 (cum) with a relative data table; (B) The goodness of fit bar plot for R2Y(cum) and Q2 (cum) with a relative data table.



Supplemental Figure 7. 3D Scatter score plot from PLS_DA and OPLS_DA modeling for differentiation of controls from *E.coli* UTI patients. (A) PLS_DA model; (B) OPLS_DA model.