

## **Supplementary Materials**

**Supplementary Fig. S1:** Quality control diagram. A and B are TIC diagrams of QC samples; C and D are EIC diagrams of internal standard in QC sample; E and F are PCA analysis of QC samples.

**Supplementary Fig. S2:** Heatmap of hierarchical clustering analysis of group AS vs HC.

**Supplementary Fig. S3:** Metabolic pathways with red/blue dots representing the differentially expressed compounds. Red means up regulation, blue means down regulation.

**Supplementary Tab. S1:** Clinical Characteristics of AS Patients.

**Supplementary Tab. S2:** Clinical Characteristics of HC Patients.

**Supplementary Tab. S3:** Positive-Differentially Expressed Metabolites.

**Supplementary Tab. S4:** Negative-Differentially Expressed Metabolites.