Supplemental Data

Supplemantal Data 1	**Suppl. Figure and Table legends (.pdf)**
Supplemental Data 2	**Suppl. Figures (.pdf)**
Supplemental Data 3	**Suppl. Tables S1, S4 and S5 (.pdf)**
Supplemental Data 4	**Suppl. Table S2 (.xlsx)**
Supplemental Data 5	**Suppl. Table S3 (.xlsx)**

Figure S1. Refined PCA of small molecular compounds that show differential signal intensities between AS patients and healthy individuals. PCA of 215 small compounds allows a clear separation between AS cases and controls (Figure 3 A). To demonstrate the validity of our approach for a diagnostic test in which the measurement of only a small number of compounds is preferred, we performed a PCA with 10 out of 215 molecular features that exhibit the largest loading (PC1) in the original PCA. The features are listed in Table S4. (1) represents the oldest individual in the control group.

Figure S2. Abundance levels (ArcSinh) of the singly charged compound at 445.2957 Da. The compound is hardly detectable in AS patients and present in abundance in most healthy individuals.

Table S1. Characteristics of subjects involved in this study

Table S2. Identified proteins and peptides in sera from AS patients and healthy individuals. 316 Protein groups were identified in all serum samples with a total of 156840 of peptide spectra matches (FDR < 2.21%).

Table S3. Up- or down-regulated proteins in AS patients. 201 Proteins were identified with ≥2 unique peptides. Label-free quantitation of these proteins (Progenesis LC-MS) was followed by LIMMA analysis and facilitated the identification of 22 up- or down-regulated proteins ($p \leq 0.05$, Benjamini-Hochberg corrected, see also Table 2).

Table S4. Up- or down-regulated small molecules in AS patient sera. 215 molecular features were detected by nLC-MS exhibiting a significant regulation between healthy individuals and AS patients. Normalized intensities for each feature are shown as Median, Maximum (Max), Minimum (Min), first and third Quartile (Q1 and Q3). These compounds were used to generate a principal component analysis (PCA) in Figure 3 A. The top 5 compounds with the highest loading along the principal component 1 (positive and negative, shaded) were used for the PCA in Figure S1.

Table S5. Up- or down-regulated small molecules differentiating the disease activity of AS patients. 65 molecular features were detected by nLC-MS exhibiting a significant regulation between the BASDAI groups 2-6, 6-8 and 8-10. Normalized intensities for each feature are shown as Median, Maximum (Max), Minimum (Min), first and third Quartile (Q1 and Q3). These compounds were used to generate a principal component analysis (PCA) in Figure 3 B.