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Quantifying Protein Quality to
Understand Protein Homeostasis
(Supplemental Data)

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A dissertation/thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

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CHAPTER 3: STRUCTURAL STABILITY OF HUMAN SERUM ALBUMIN IS MODIFIED IN RHEUMATOID ARTHRITIS

CH3-Supplemental Data 1 (.zip): HDC Results/Simulation

- The zip file includes 47 HDC results (.csv) exported from DSC raw files. Each HDC result file contains seven measurements for each DSC run: temperature (°C), power (μW), time(s), pressure (atm), scan rate (°C/min), analysis data (excess molar heat capacity (C_{pex})), and corrected data (normalized C_{pex}, normalization explained in the Methods section).

CH3-Supplemental Data 2 (.xlsx): Protein Quantification

- **protein-peptide:** the peptide area exported from LFQ from PEAKs Studio for the 49 samples. This is used for protein quantification, and PTM analysis.
- **Filter:** The filters applied for LFQ analysis.

CH3-Supplemental Data 3 (.xlsx): PTM Results for HSA

- **PTM Results for HSA**
 - **ProteinProspector:** Lists the PTM search result on HSA.
 - Peptide information: Lists peptide sequence, peptide start position, peptide end position, peptide theoretical mass, precursor m/z, precursor mass, and precursor mass.
 - First/Second Modification: Lists the amino acid, the position, the mass shift value of the modification, as well as SLIP score (a quality merit of the modification)
 - Hit: List if the modified peptide is observed in a sample. If it is present, the sample name is record in the same row of the peptides. The analysis only returns present or not, thus PEAKs studio is used for further quantification.
 - **Customized PTM search:** Lists the name, m/z shift, modified AA for the PTM put in the database search step of PEAKs studio analysis.
 - **Albu_ptm profile:** The data from PTM profile of PEAKs Studio SPIDER analysis. It lists all PTM observed on HSA, and the modification site. The peptide sequence window, the modified amino acid (AA), the occurrence of the same modified AA in the dataset, the modified site on the protein, the occurrence of the same modified site in the dataset, best-10logP, best ion intensity (%), and number of hit across 49 samples.

CH3-Supplemental Data 4 (.xlsx): AEBSF sites on HSA

- **T-test:** Lists t-test results between RA and non-RA subjects, as well HPR and LPR subjects, showing significance between RA and non-RA subjects in each comparison. The average intensity of the sum of all of AEBSF modification sites on HSA of each sample, for RA and non-RA, as well as HPR and LPR, is shown. A t-test was also performed between groups for modification sites in clusters 1, 2, and 3.
- **AEBSF_HSA (site):** This dataset lists the structure characteristic of the 41 AEBSF sites on HSA, including association with the cluster groups from Figure 4B, HC order from Inferno, site position from Uniprot, site position from PDB ID 1N5U, HSA domain, HSA subdomain, amino acid (AA), secondary structure (SS), surface accessible surface area (SASA) score, number of peptides used for the quantification of the site, peptide sequence, and the intensity from each sample. (The intensity here used the area from supplemental data 3. Only peptides from HSA and with AEBSF modifications are

retained. The area of peptides that have same AEBSF modification site are combined (the number of peptides is used for combination is listed in column #peptide combined). After consolidation, site that have less than 12 hits are removed. Note that the sequence/start/end for sites that used more than 1 peptides are just representative. The intensity is also used for Inferno analysis).

AEBSF_HSA_(cluster site) : A list of all samples, with their groups (RA/non-RA and HPR/LPR), as well as the intensity sum of AEBSF modification for each modification site in cluster C1, C2, C3 on HSA.

CH3-Supplemental Information (.docx) MS2 spectra for PTM on HSA

CHAPTER 4: QUANTIFYING IN SITU STRUCTURAL STABILITIES OF HUMAN BLOOD PLASMA PROTEINS USING A NOVEL IODINATION PROTEIN STABILITY ASSAY (IPSA)

CH4-Supporting Data 1(xlsx)- IPSA and SPROX's label and fitting efficiency

CH4-Supporting Data 2(xlsx)- Statistics test results for reproducibility, slope tendency, $C_{1/2}$ and SASA distribution, and $C_{1/2}$'s correlation to structural parameter.

CH4-Supporting Data 3 (xlsx)- $C_{1/2}$ value and structural parameters for each site measured

CH4-Supporting Data 4 (xlsx)-Merged C_{Half} output (combined label site) and the average $C_{1/2}$ for serum protein

CH4-Supporting Data 5 (xlsx)- Structural parameters of 17 different transferrin

*Detailed description for the columns and rows can be found in the note spreadsheet in the excel files.