

NMR Spectroscopic Approach Reveals Metabolic Diversity of Human Blood Plasma Associated with Protein-Drug Interaction

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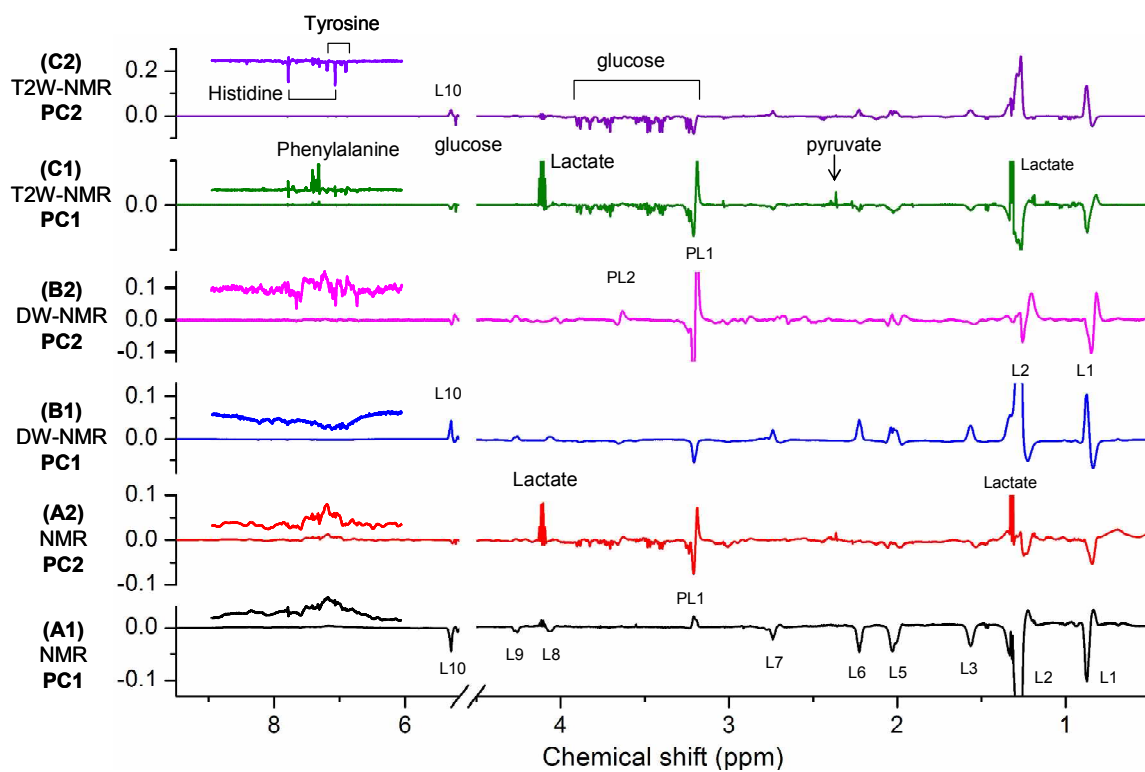


Figure S2. Linear PCA loadings plots (PC1 & PC2) based on the NMR (A1 & A2), DW-NMR (B1 & B2) and T2W-NMR (C1 & C2) datasets of the blood plasma samples without and with ibuprofen. The major components contributing to the separation of PCA scores plot (Figure 2B-2D) were labeled.

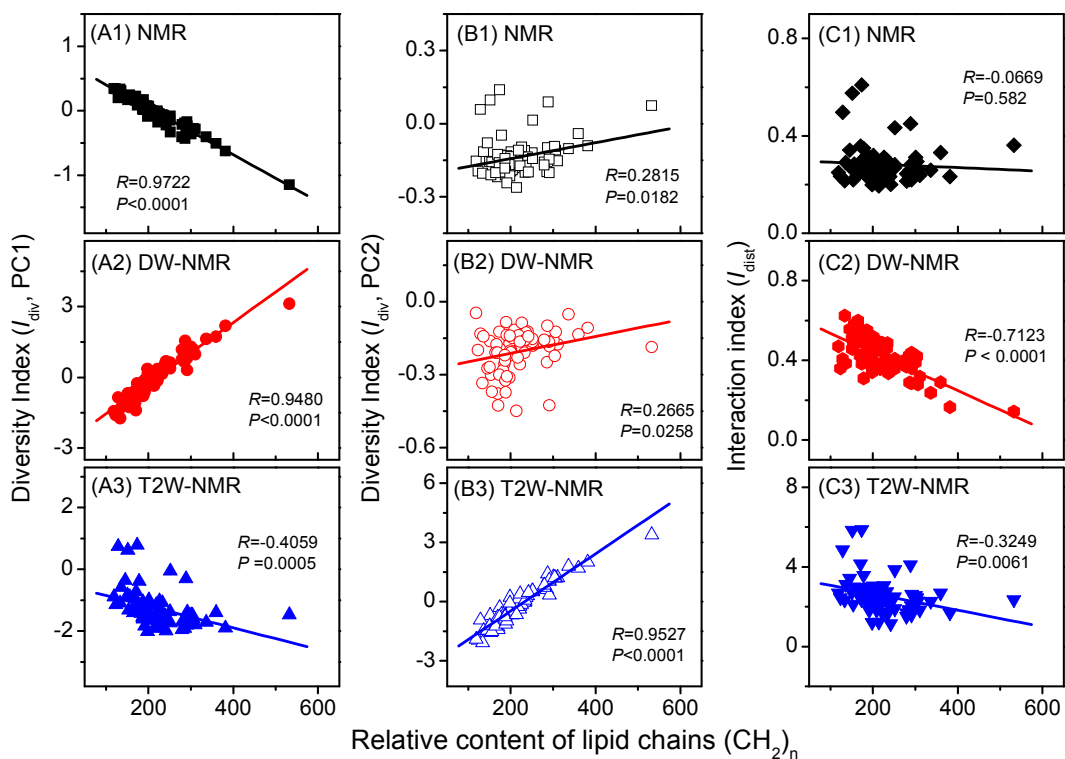


Figure S3. Plots of the diversity indexes defined by PC1 (A1-A3) and PC2 (B1-B3), and the interaction index (C1-C3) as function of the relative content of lipid chains (CH₂)_n, based on PCA of NMR (A1, B1, C1), DW-NMR (A2, B2,C2) and T2W-NMR (A3, B3, C3) datasets. Linear fittings (line symbols) and the fitting parameters (R , P) were also given.