

NMR-based metabolomics in differential diagnosis of chronic kidney disease (CKD) subtypes

Supplementary Material

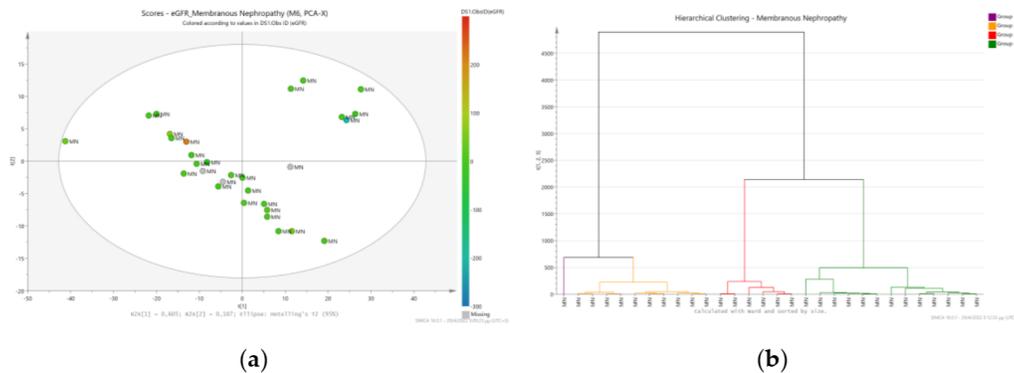


Figure S1. Membranous Nephropathy (MN) ^1H NMR urinary metabolic profile. Unsupervised visualization of cluster tendency. (a) PCA 2D scores plot of MN applied on the data set of 30 ^1H CPMG NMR urine spectra; spheres are colored according to the eGFR value via heatmap visualization. (b) PCA-Hierarchical Clustering on the same MN metabolic NMR profiles.

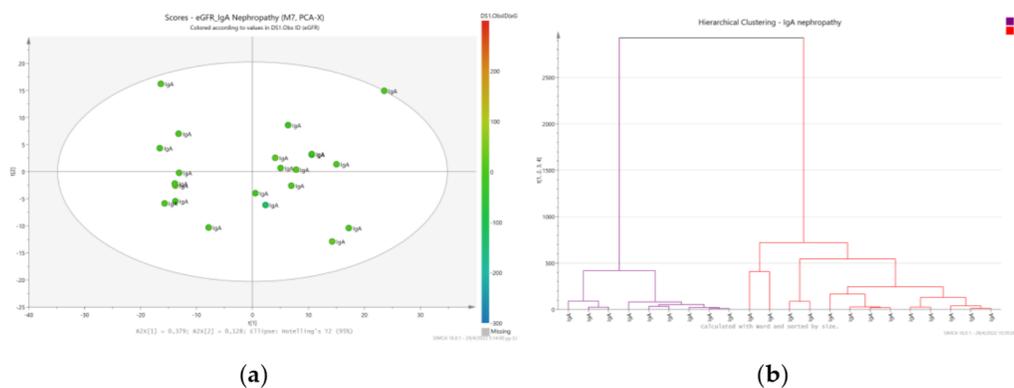
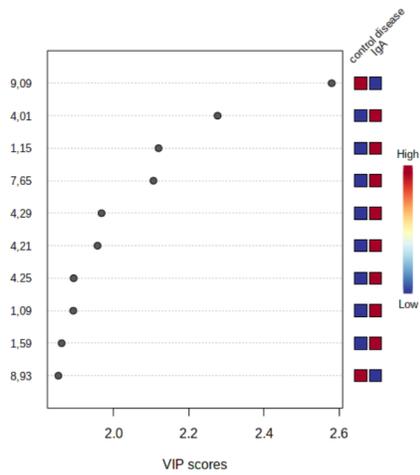
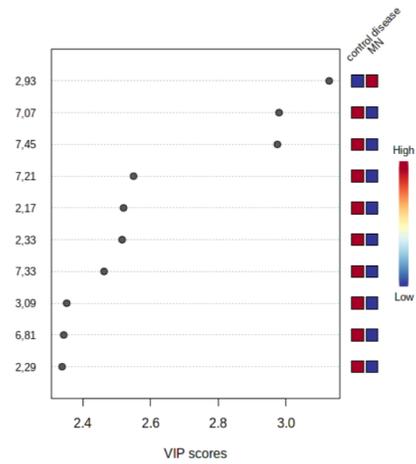


Figure S2. IgA Nephropathy (IgAN) ^1H NMR urinary metabolic profile. Unsupervised visualization of cluster tendency. (a) PCA 2D scores plot of IgAN applied on the data set of 22 ^1H CPMG NMR urine spectra; spheres are coloured according to the eGFR value via heatmap visualization. (b) PCA-Hierarchical Clustering of the IgAN metabolic NMR profiles.

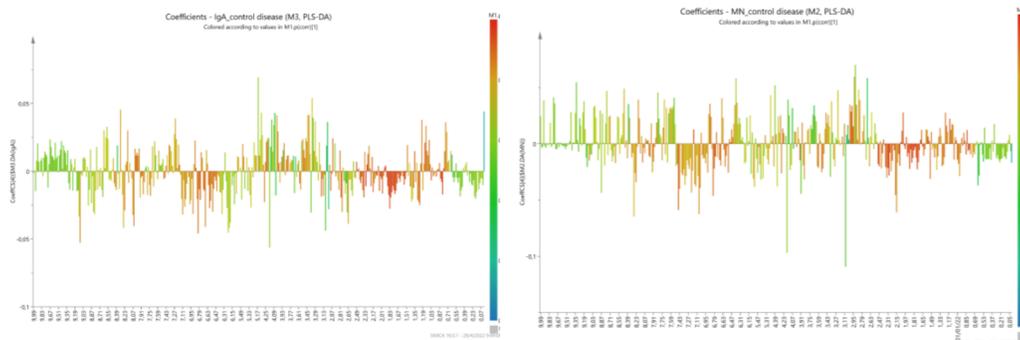


(a)

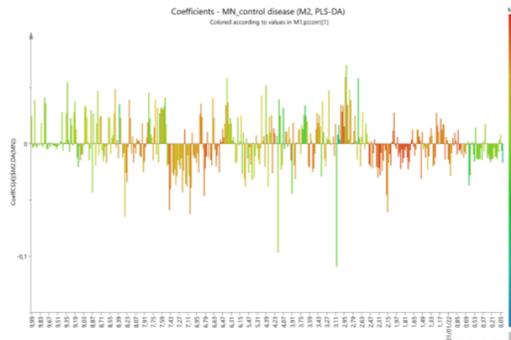


(b)

Figure S3. Statistically significant features of the glomerulonephritis subtypes comparison with the control disease patients. The first 10 VIP scores of the first PLS-DA Latent Variable indicating the variables of importance between (a) IgAN and (b) MN and control disease patients' metabolic profile respectively.



(a)



(b)

Figure S4. PLS-DA coefficients' plot for the classification which reveals the relative intensities between the two examined groups. (a) IgAN and control disease and (b) MN and control disease patients. The color-coded correlation coefficients indicate the significance of the metabolites in terms of their contribution to the separation between the two groups.