

Supplementary File 1

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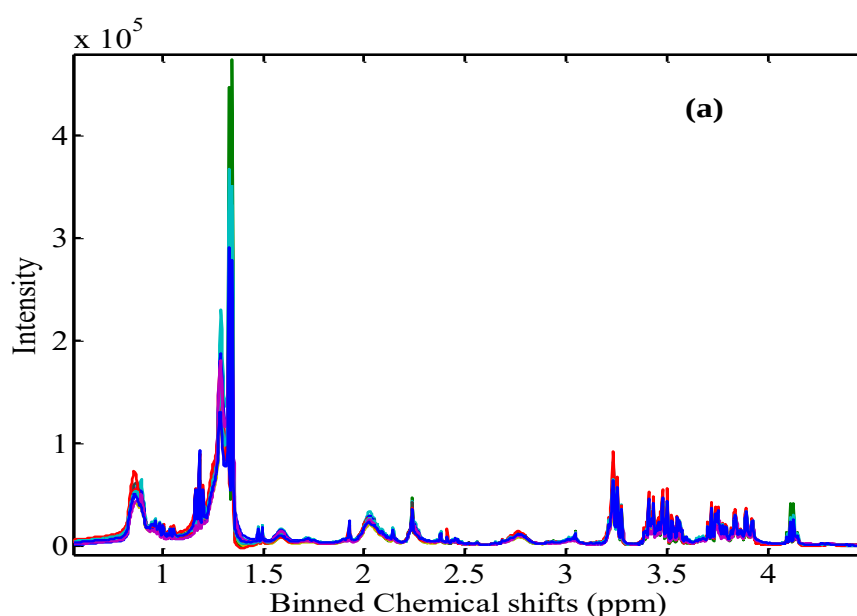
The assessment of metabolite alteration induced by –OH functionalized multi-walled carbon nanotubes in mice using NMR-based metabonomics

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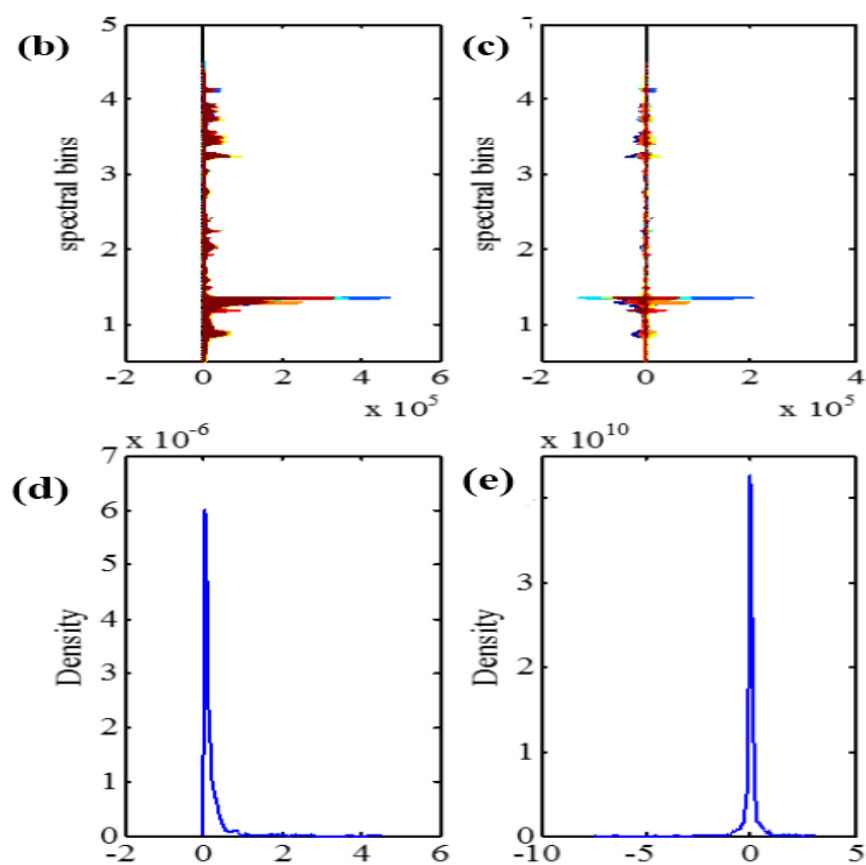


Figure S1. (a) ^1H NMR data after preprocessing. (b, c) bar and (d, e) density plots of plasma samples (b, d) before and (c, e) after mean centering. In bar plots (on the top) the concentration distributions were shown, while kernel density plots (on the bottoms) shows the overall concentration distributions based on Pareto scaling estimation.

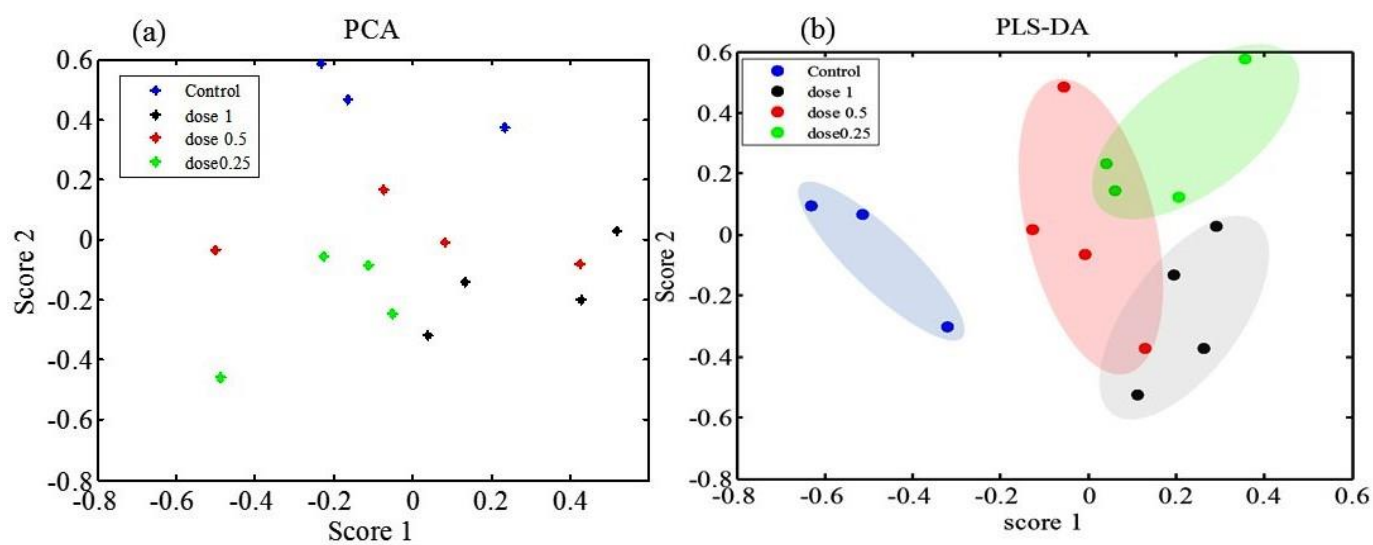


Figure S2. Estimated scores applying (a) PCA and (b) PLS-DA on data sets. As can be seen a good spatial separation of samples based on doses of MWCNTs-OH is observed by PLS-DA clearly

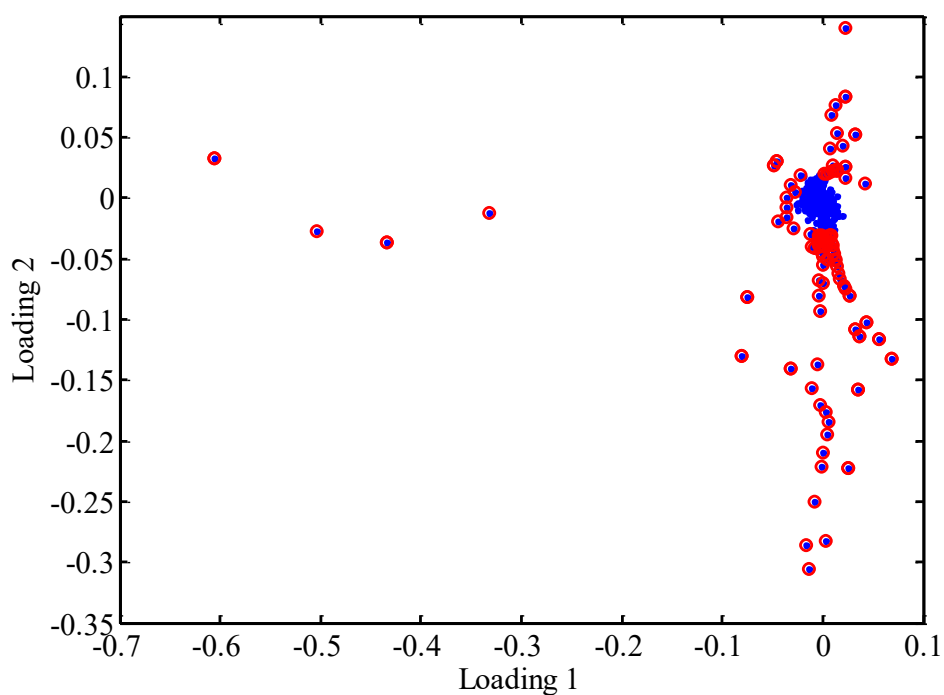


Figure S3. Estimated loadings applying PLS-DA on NMR data. The red points in figure represent the points which correspond to chemical shifts responsible for separation of groups in score plot.