

NMR metabolomics in serum fingerprinting of Schizophrenia Patients in the Serbian cohort

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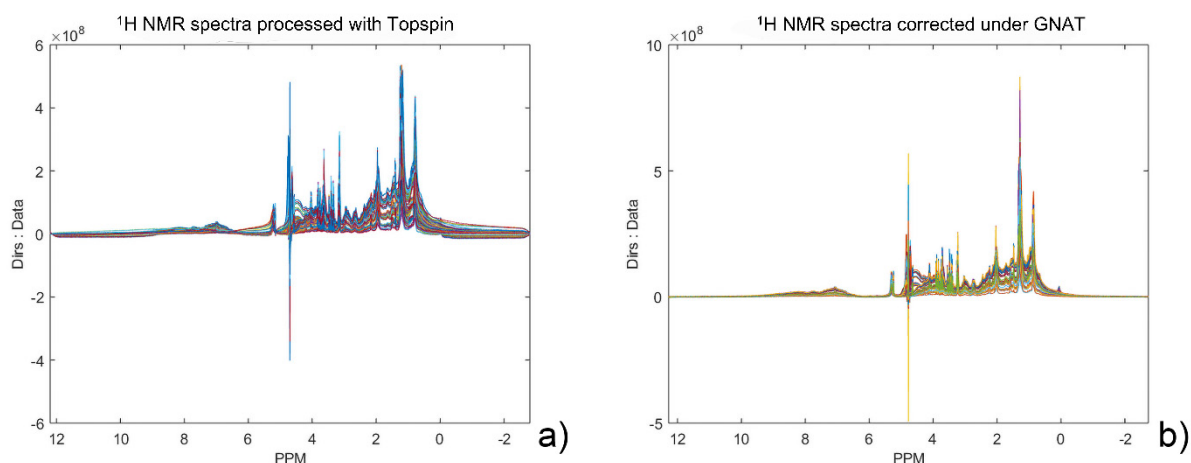


Figure S1. (a) ^1H -NMR spectra, processed using the Bruker Topspin software. (b) The same spectra with the phase of 0th order, corrected under the GNAT program.

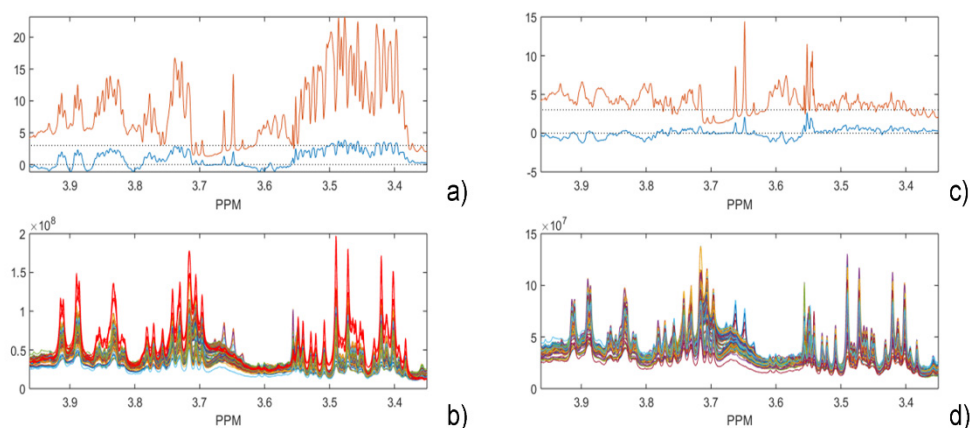


Figure S2. a) Results for skewness and kurtosis in the area of spectra with significant discrepancies from common value for normal distribution (0 for skewness and 3 for kurtosis); b) NMR spectra in the region, where spectra colored in red indicate potential outliers. c) Results for skewness and kurtosis in the area of spectra after removing the samples identified as potential outliers. The horizontal dotted lines on both Figures are passing/going through the given values for skewness and kurtosis (0 and 3, r) of any univariate normal distribution. d) NMR spectra in the corresponding region after removing the spectra colored in red (b).

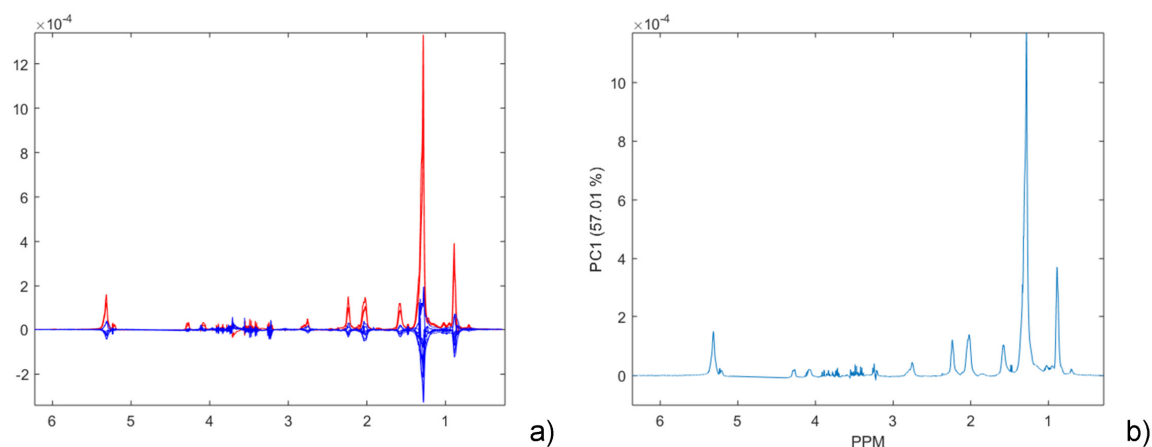


Figure S3. a) Mean-centered NMR spectra referring to the samples marked with ellipses in Figure 1a, in red color;

b) Several NMR spectra of samples that originate from the central part of the score plot presented in Figure 1a are given in blue.

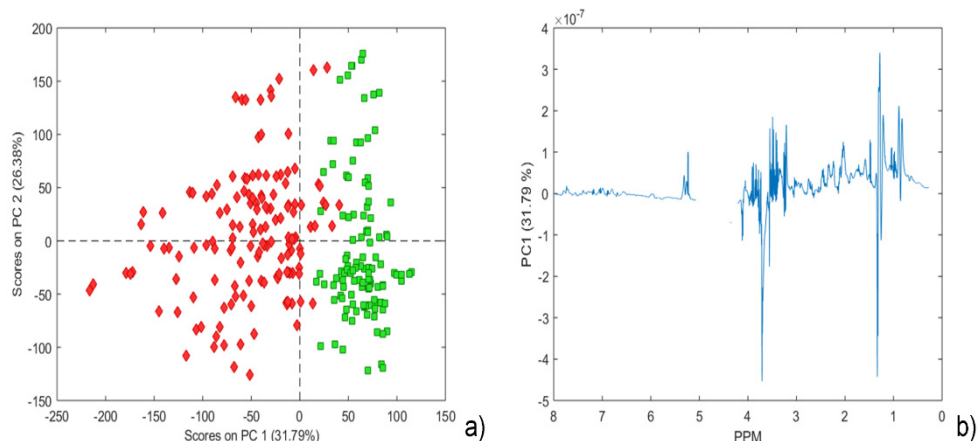


Figure S4. a) Score plot of PCA model presented in PC 1 vs. PC2 components. Scaling and centering were accomplished with autoscaling; b) Corresponding loading plot of PC 1 component.

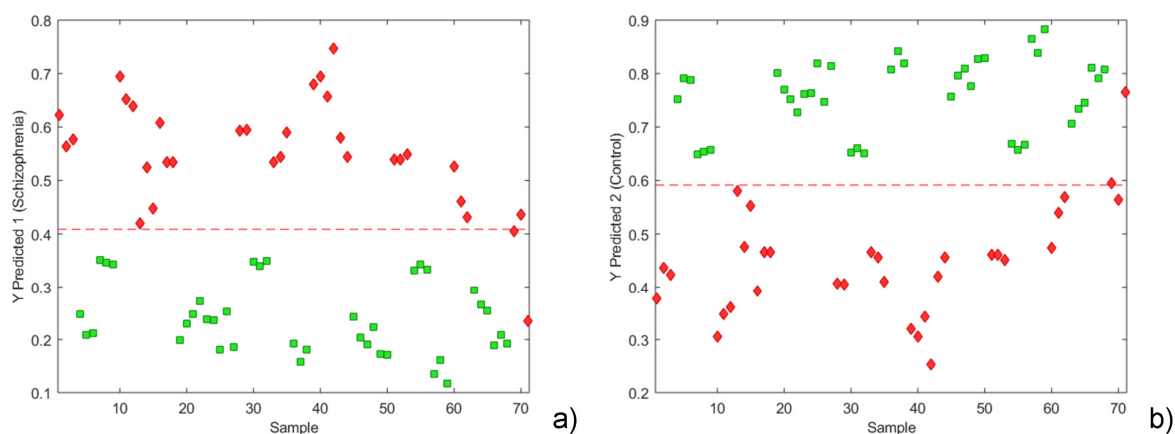


Figure S5. a) Y Predicted for the class 'Schizophrenia' and b) Y Predicted for the class 'Control' from external test data set, using autoscaling.

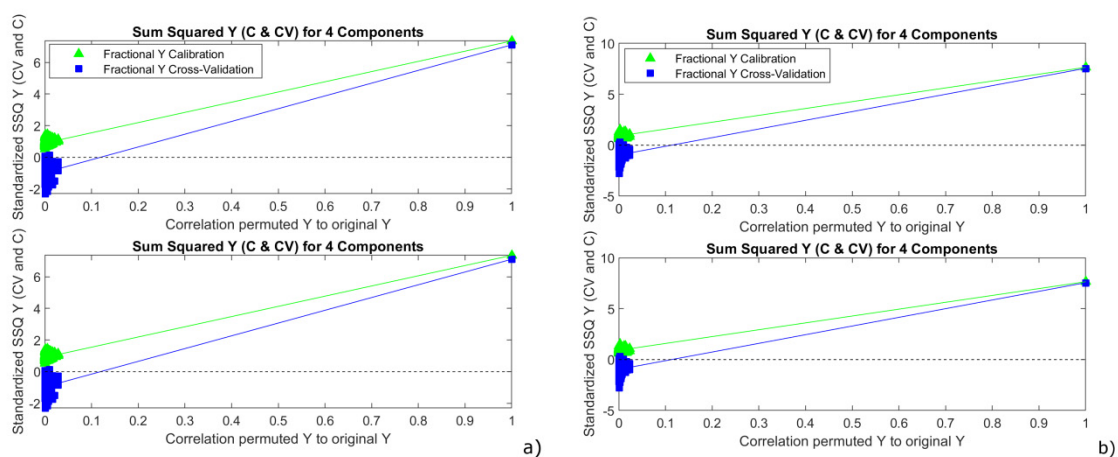


Figure S6. Fractional Y-variance captured for self-prediction (calibration) and cross-validation versus the correlation of the permuted Y-block to the original Y-block for 4 LV component models of **a)** OPLS-DA model using autoscaling and **b)** OPLS-DA model using class centroid centering and scaling.