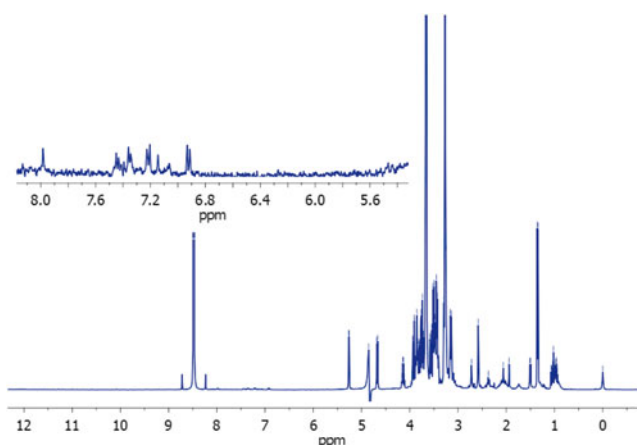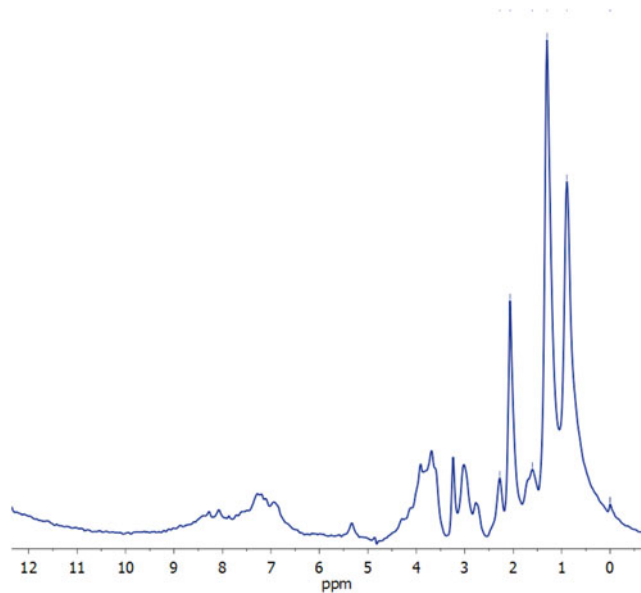# Supplementary Data

The *N*-way Partial Least Squares Discriminant Analysis

The ensemble of hydrogen nuclear magnetic resonance (^{1}H NMR) spectra was resumed in a cube of data (X) with a trilinear structure (samples × time × variables). N-way partial least squares (NPLS) is an extension of the PLS algorithm for higher order data; the method preserves the trilinear data structure and produces vectors, which score covariance maximized with the dependent variable (Bro, 1996). NPLS can be extended to discriminant analysis (NPLS-DA) with the response matrix replaced with a dummy vector containing zero and ones. NPLS-DA decomposes X into a set of weights represented by vectors *wj* and *wk*, and scores represented by vectors *t*. Each vector *t* represents a sample variation in relation to total variation of data (scores). The vectors *wj* represent the weight applied to each variable to provide the values of *t*-scores for a given sample. The *wk* summarizes the temporal variation of the variables measured in relation to average trajectories. The weights and scores are obtained by an iterative process in which the sum of squared errors is minimized. The scores are determined successively to obtain maximum covariance with the dependent variable (y) (Supplementary Fig. S5).


SUPPLEMENTARY FIG. S1. Representative T$_2$-edited ^{1}H NMR spectra model for overweight subjects before RYGB acquired using CPMG and water presaturation (PRESAT). The *insert* shows the aromatic region magnified 100 times. ^{1}H NMR, hydrogen nuclear magnetic resonance; CPMG, Carr–Purcell–Meiboom–Gill pulse sequence.


SUPPLEMENTARY FIG. S2. Representative diffusion-edited ^{1}H NMR spectrum model for overweight subjects before RYGB acquired using a bipolar pulse pair-longitudinal eddy current delay pulse sequence and WATERGATE 3-9-19.
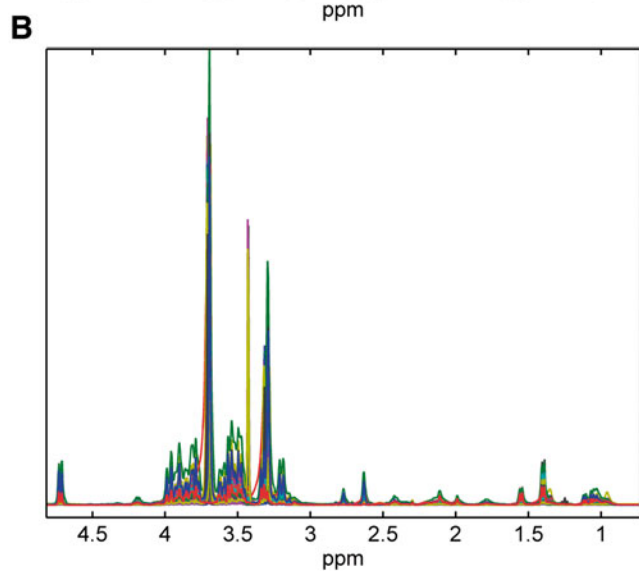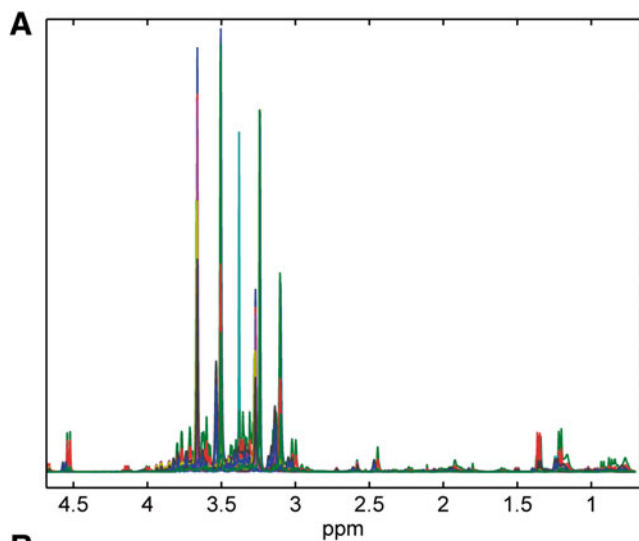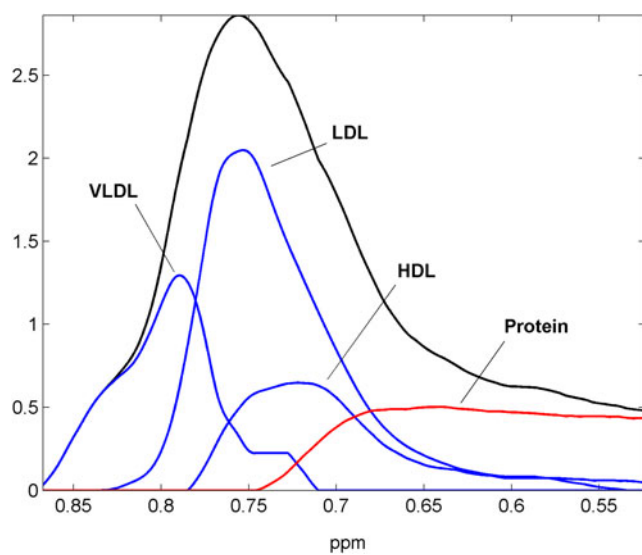
SUPPLEMENTARY FIG. S3. Ensemble of 360 T$_2$-edited ^{1}H NMR spectrum **(A)** before and **(B)** after the ICOSHIFT alignment and Sousa's bucket.
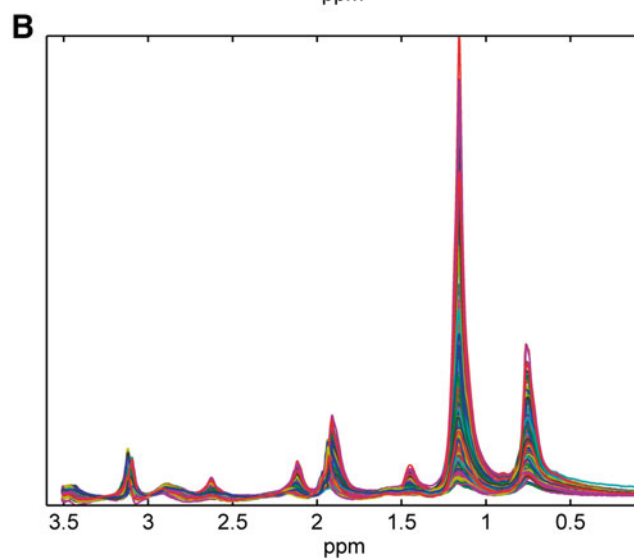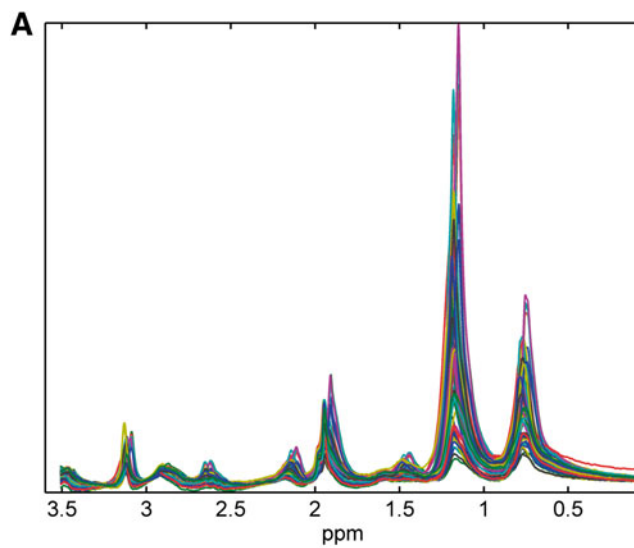

SUPPLEMENTARY FIG. S4. Ensemble of 360 diffusion-edited ^{1}H NMR spectrum **(A)** before and **(B)** after the ICO-SHIFT alignment and Sousa's bucket.
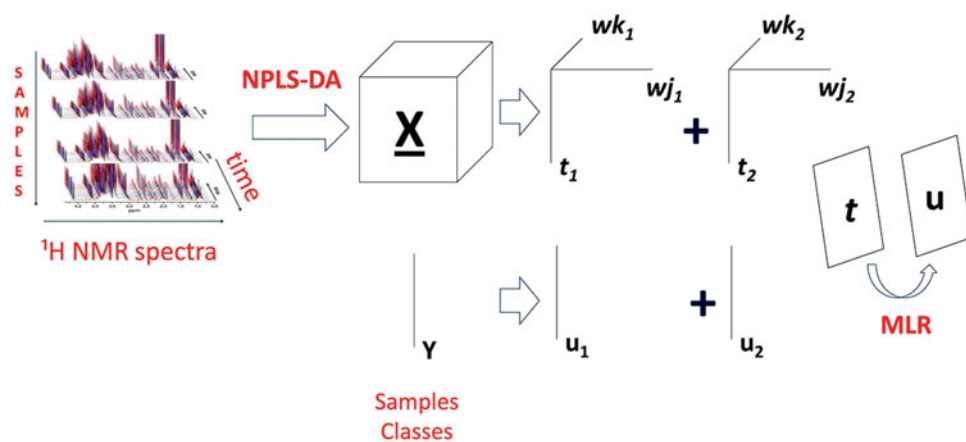
SUPPLEMENTARY FIG. S5. The NPLS-DA overview. NPLS-DA, *N*-way partial least squares discriminant analysis.

SUPPLEMENTARY FIG. S6. MCR deconvolution of methyl resonances from lipoprotein. HDL, high-density lipoprotein; LDL, low-density lipoprotein; MCR, multivariate curve resolution; VLDL, very low-density lipoprotein.
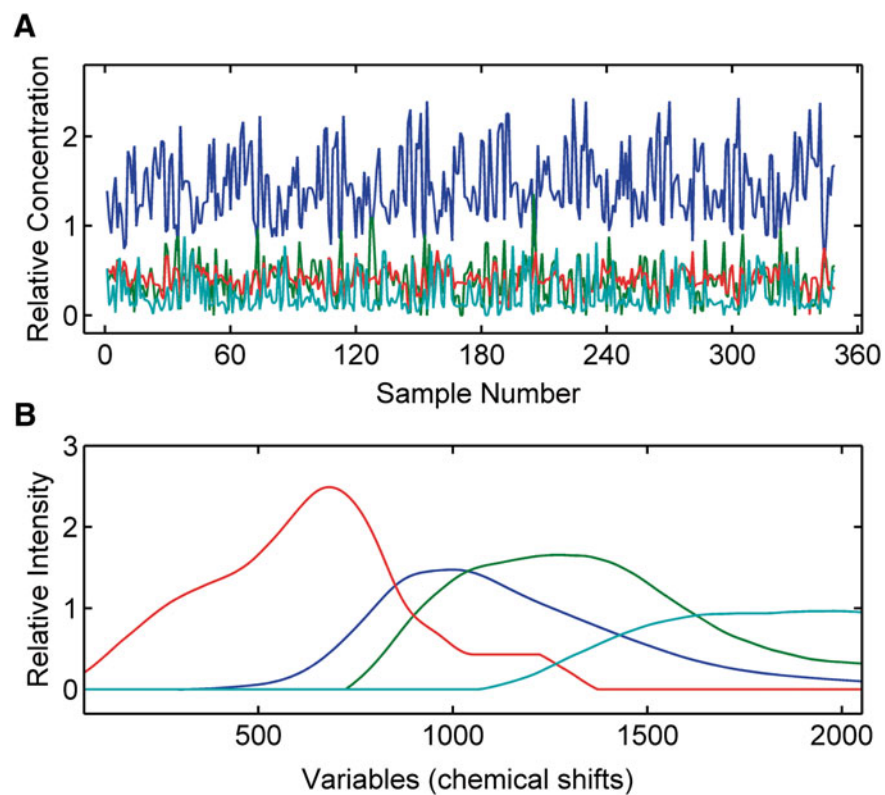
SUPPLEMENTARY FIG. S7. **(A)** Relative concentration achieved by MCR applied to methyl resonance from diffusion-edited ^{1}H NMR spectrum; **(B)** curves optimized by MCR. A curve representing protein was included to accommodate baseline variations associated to protein content.