Figure S1 : PCA scores scatter plot obtained from ^{1}H-NMR urinary spectra of control (blue) and autistic (red) children. The NMR intensity bins were scaled to the total spectral intensity.

R2X[1] = 0,137005   R2X[2] = 0,0986927
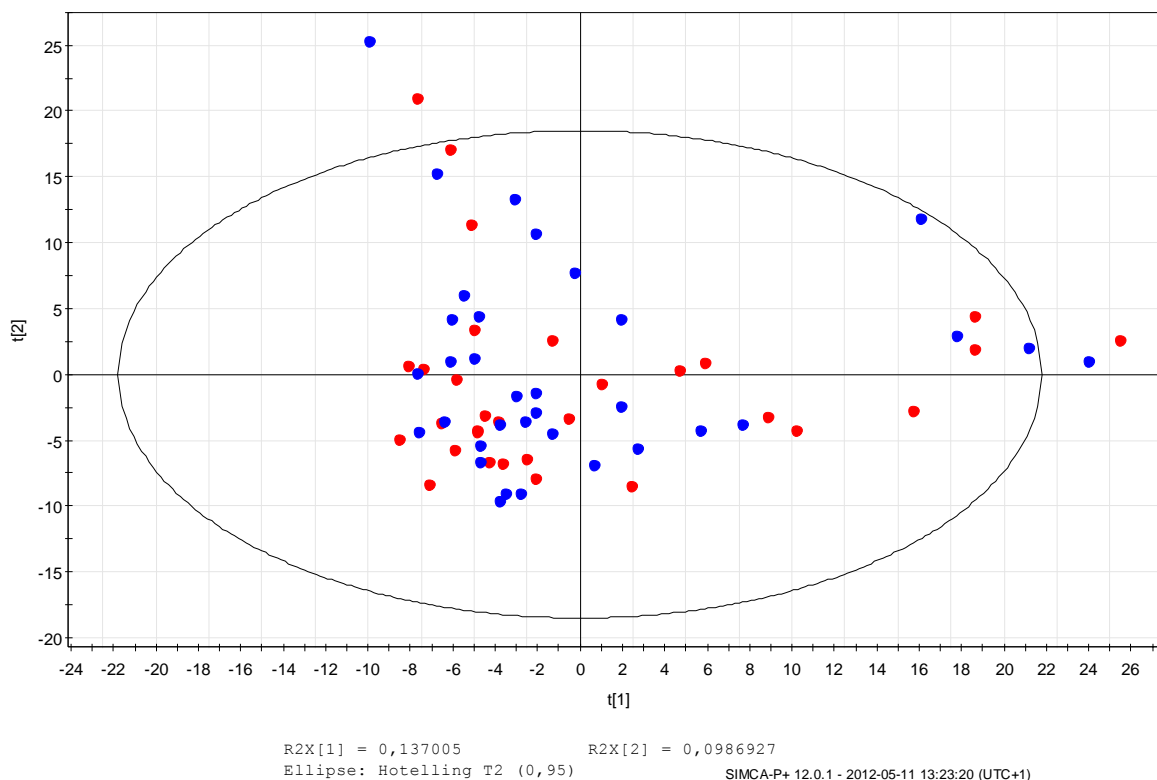Ellipse: Hotelling T2 (0,95)

SIMCA-P+ 12.0.1 - 2012-05-11 13:23:20 (UTC+1)

Figure S2: Validate model plot of the PLS-DA obtained with the ^{1}H NMR data to test the overfitting of the data (intercepts Q2=(0.0, -0.137) R2=(0.0, -0.258)).
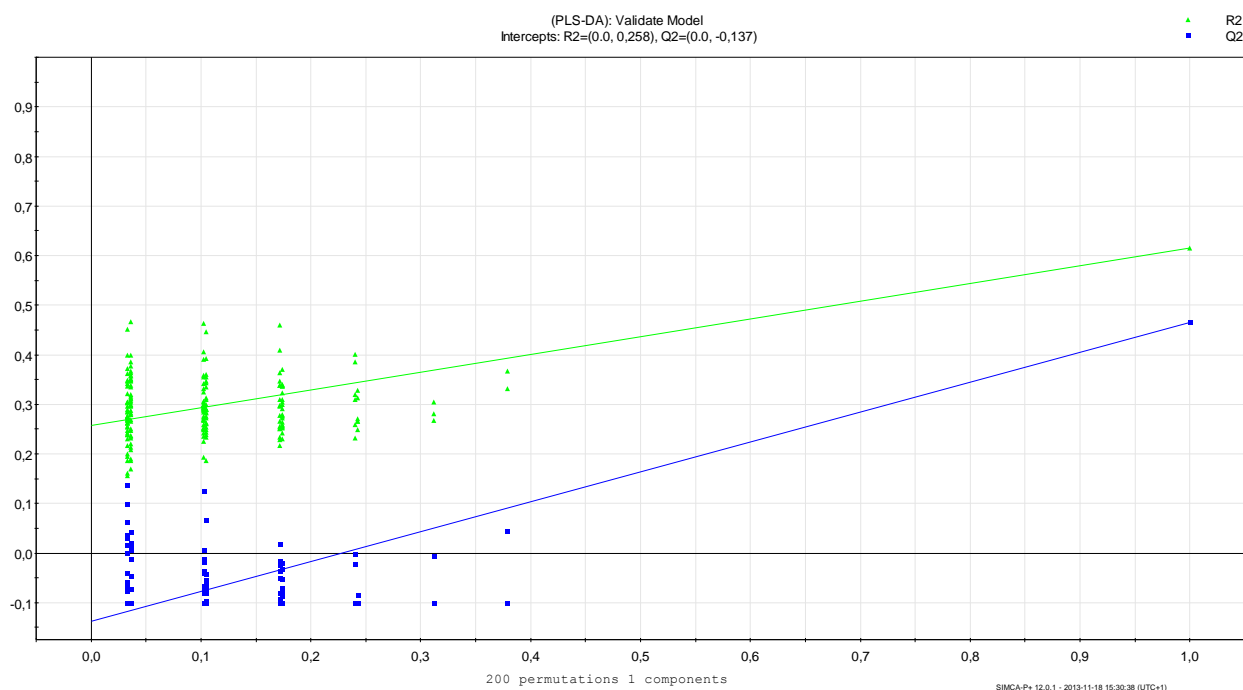

Figure S3: Contribution plot obtained from ^{1}H-NMR urinary spectra. Spectral variables discriminating control (positive variables) and

autistic (negative variables) children are summarized. (R^2Y(cum)=0.70, Q^2=0.51, CV-ANOVA p=8.3710^{-8}).

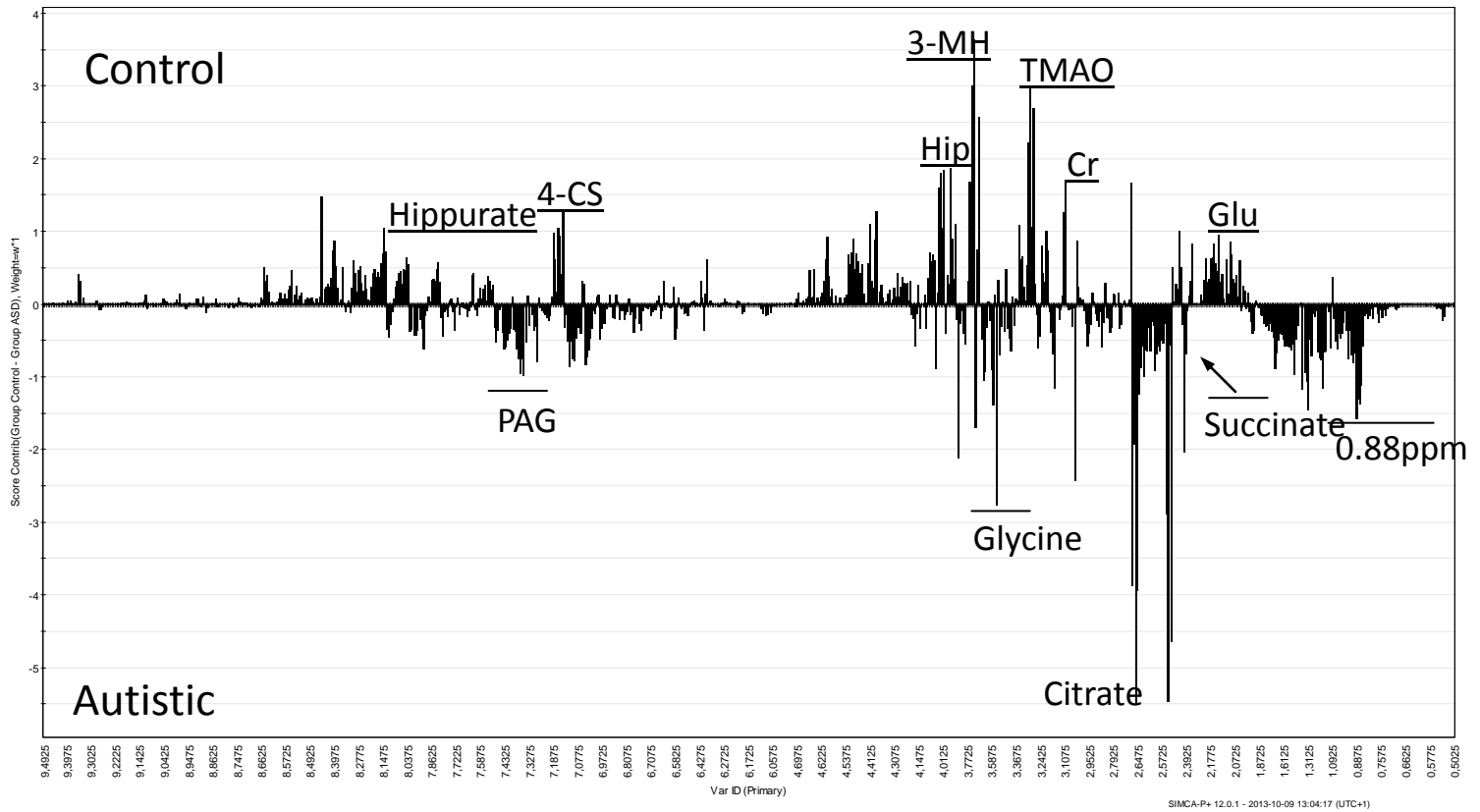(PAG: phenylacetylglutamine, Hip: hippurate, Gly: glycine, 3-MH: 3methyl histidine, glu: glutamate).

Figure S4: OPLS-DA scores scatter plot obtained from ^{1}H-NMR urinary spectra of control (white circle) and autistic (black square) children. The NMR intensity bins were scaled to the creatinine spectral intensity. (R^2X(cum)=0.356, R^2Y(cum)=0.69, Q^2=0.36)
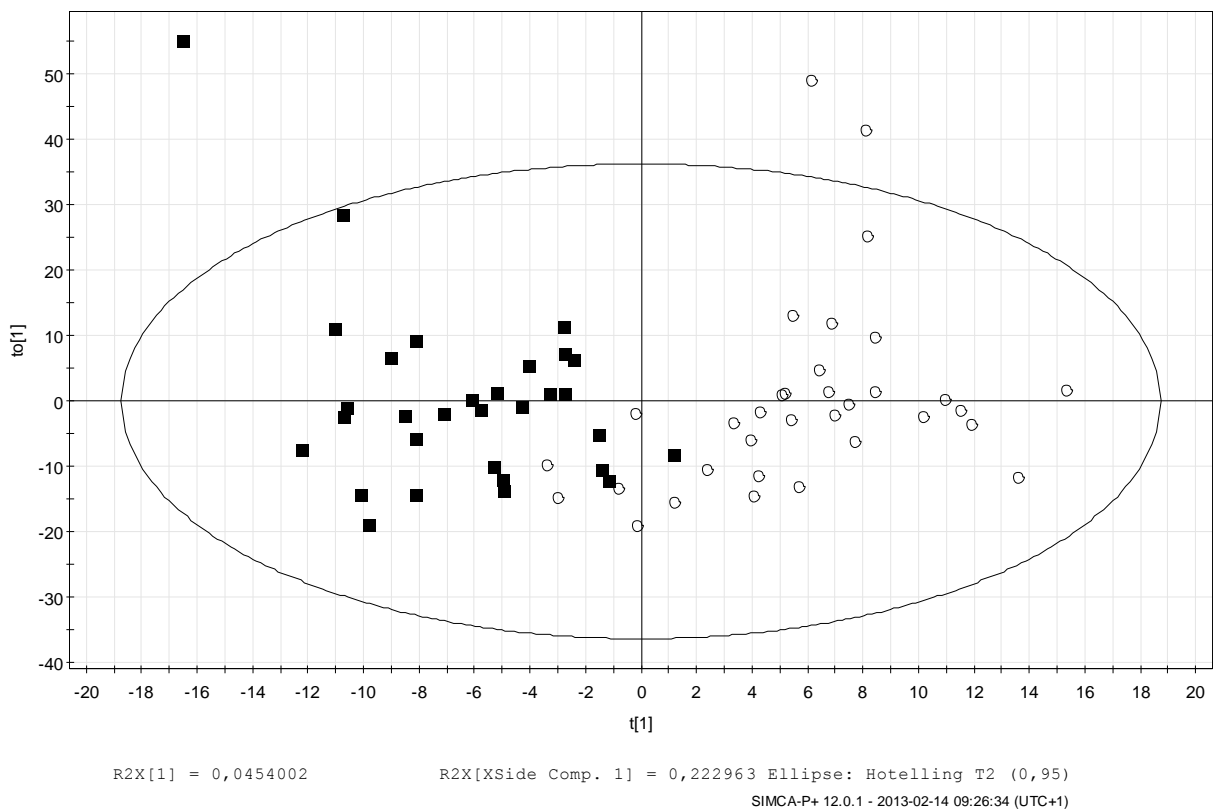
Figure S5: Receiver-operating characteristic (ROC) curves and area under curve (AUC) according to the three OPLS-DA models (a : 1H NMR data, b: 2D HSQC NMR cross-correlation, c: combined 1H NMR and HSQC NMR cross-correlation).