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.

Figure S2: Validate model plot of the PLS-DA obtained with the $^1$H NMR data to test the overfitting of the data (intercepts $Q^2=(0.0, -0.137)$ $R^2=(0.0, -0.258)$).

Figure S3: Contribution plot obtained from $^1$H-NMR urinary spectra. Spectral variables discriminating control (positive variables) and autistic (negative variables) children are summarized. ($R^2 Y_{(cum)}=0.70$, $Q^2=0.51$, 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. 

$(R^2_X(cum)=0.356, R^2_Y(cum)=0.69, Q^2=0.36)$
**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).