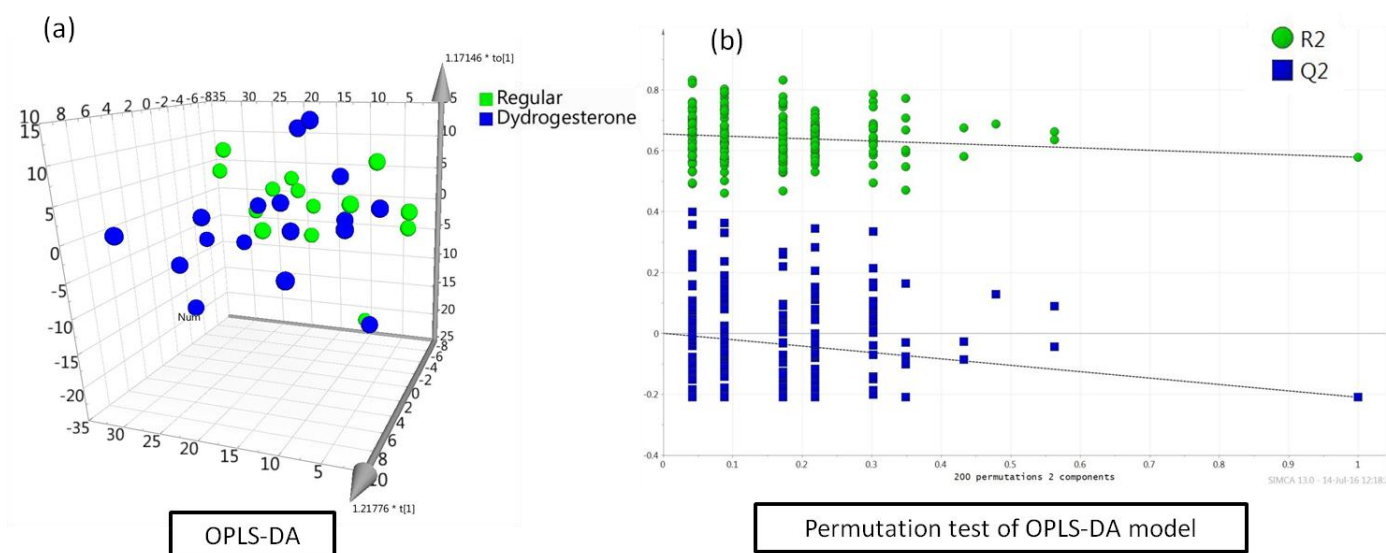
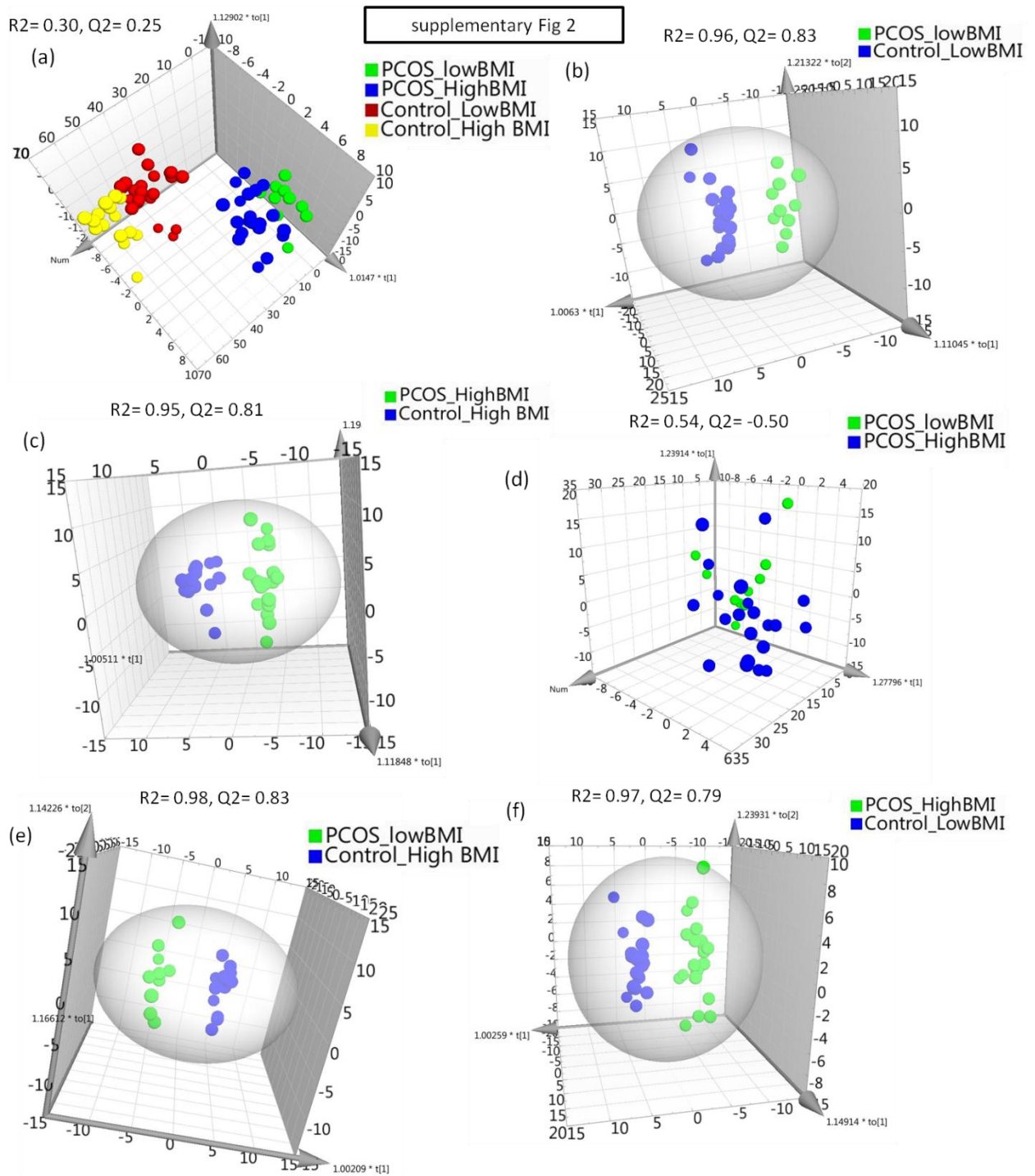


Supplementary material

supplementary Fig 1

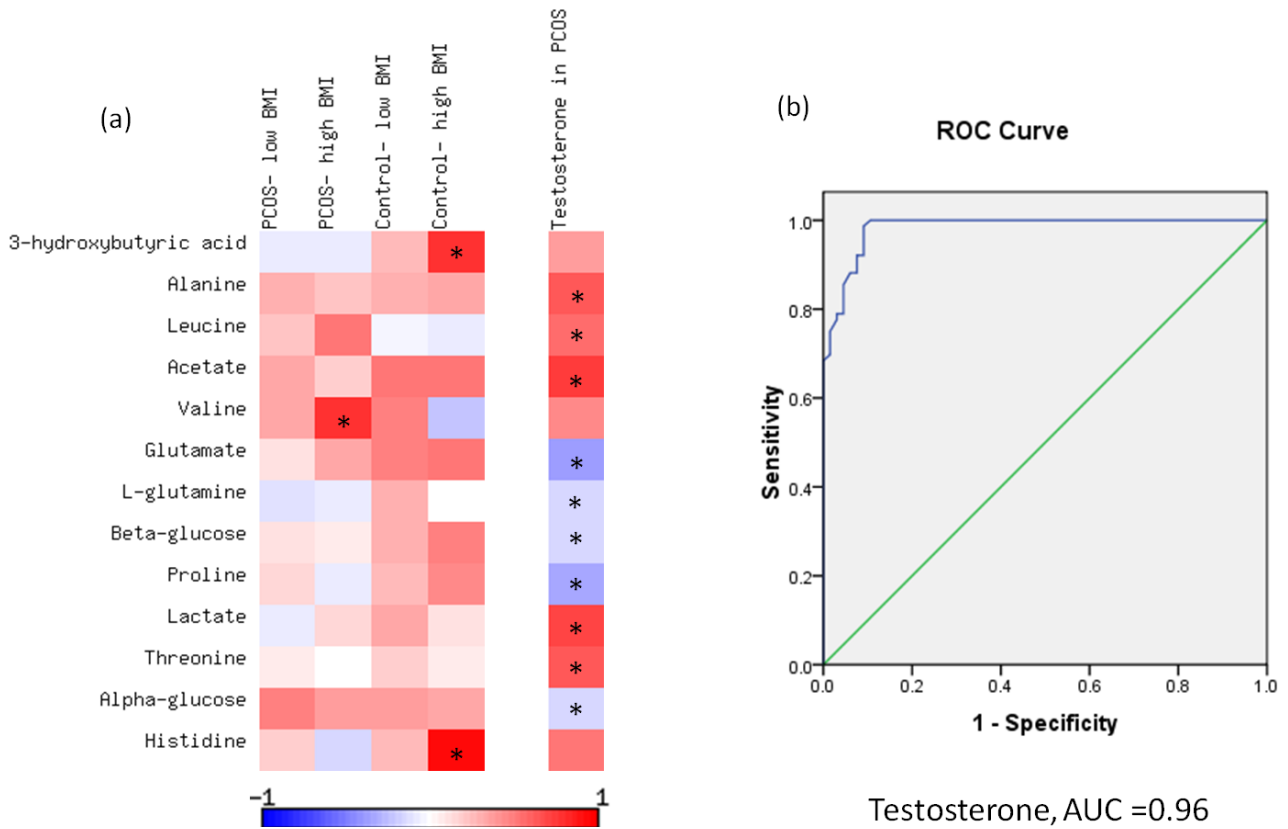


Supplementary fig1: Score scatter plot of (a) OPLS-DA showing mixed patterns and no clear discrimination between PCOS women with regular menstrual cycle (green) and dydrogesterone administered PCOS patients (blue) (b) The statistical significance of the OPLS-DA model is checked using permutation test ($n = 200$). The R2 and Q2 values of the obtained true model are on the extreme right-hand side of the plot. The R2 and Q2 values of the original model in the validation test exhibited low values than those of the randomly permuted models



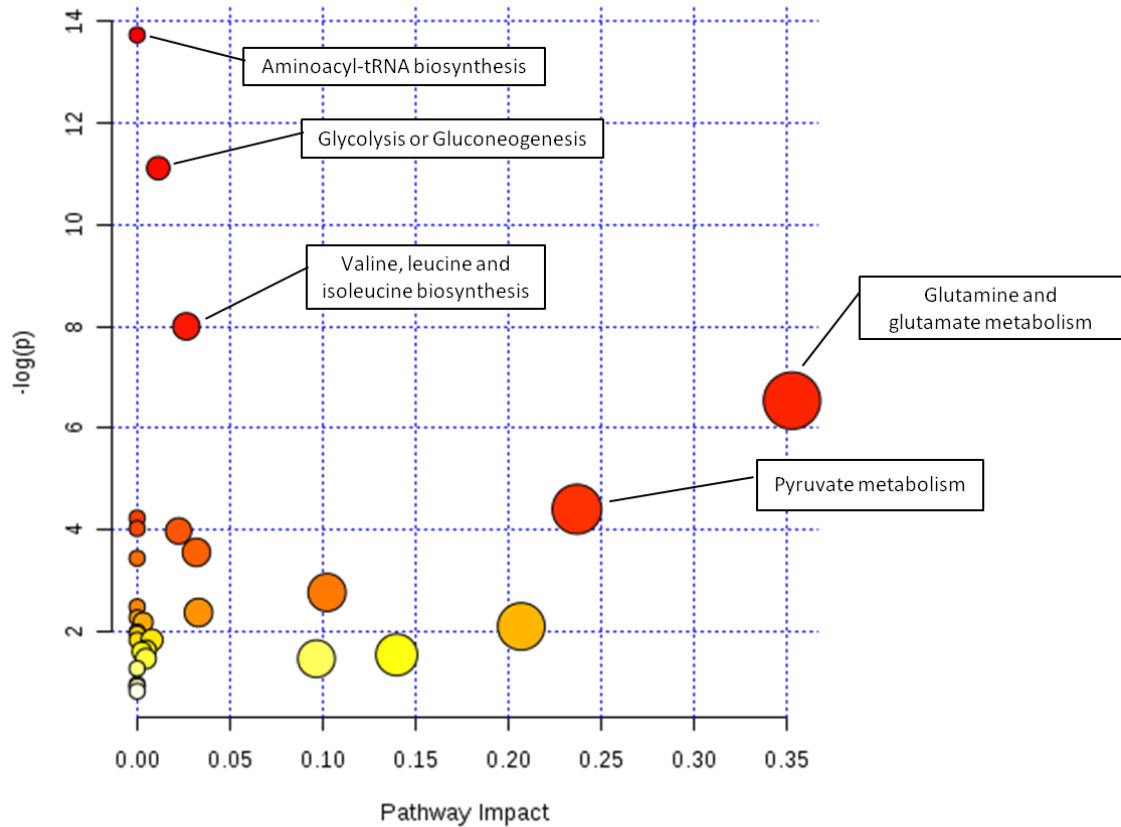
Supplementary fig2: Score scatter plots of OPLS-DA for (a) low BMI PCOS (green), high BMI PCOS (blue), low BMI Controls (red) and high BMI Controls (yellow); (b) low BMI PCOS (green) vs low BMI Controls (blue); (c) high BMI PCOS (green) vs high BMI Controls (blue); (d) low BMI PCOS (green) vs high BMI PCOS (blue); (e) low BMI PCOS (green) vs high BMI Controls (blue); (f) high BMI PCOS (green) vs low BMI Controls (blue)

supplementary Fig 3



Supplementary fig3: (a) Correlation of identified major metabolites with BMI (low and high BMI subgroups from both the PCOS and control groups) and testosterone levels of PCOS patients are represented as a heatmap corresponding to a matrix of Pearson's correlations. Marked correlations are significant ($p < 0.05$); (b) ROC curve for testosterone with AUC value of 0.96

supplementary Fig 4



Supplementary fig4: Metabolic pathway analysis (MetPA) of PCOS patients. MetPA generated pathway impact score indicates the potential pathways altered in women with PCOS. MetPA calculates the pathway impact based on the matched metabolites normalized by importance measures of all metabolites in each pathway. Pathway impact represents the potentially altered metabolic pathways. The most impacted pathways with high significance score are highlighted. MetPA generated pathway indicates alterations in aminoacyl-tRNA biosynthesis, glycolysis/gluconeogenesis, valine/leucine/isoleucine biosynthesis, glutamine/glutamate metabolism and pyruvate metabolism

Supplementary Table 1: The pathway analysis shows potential pathways involved PCOS

	Total	Expected	Hits	Raw p	Holm p	FDR	Impact
Aminoacyl-tRNA biosynthesis	75.00	0.41	6.00	0.00	0.00	0.00	0.00
Glycolysis or Gluconeogenesis	31.00	0.17	4.00	0.00	0.00	0.00	0.01
Valine, leucine and isoleucine biosynthesis	27.00	0.15	3.00	0.00	0.03	0.01	0.03
D-Glutamine and D-glutamate metabolism	11.00	0.06	2.00	0.00	0.11	0.03	0.35
Pyruvate metabolism	32.00	0.17	2.00	0.01	0.93	0.19	0.24
Propanoate metabolism	35.00	0.19	2.00	0.01	1.00	0.19	0.00
Nitrogen metabolism	39.00	0.21	2.00	0.02	1.00	0.19	0.00
Valine, leucine and isoleucine degradation	40.00	0.22	2.00	0.02	1.00	0.19	0.02
Starch and sucrose metabolism	50.00	0.27	2.00	0.03	1.00	0.25	0.03
Synthesis and degradation of ketone bodies	6.00	0.03	1.00	0.03	1.00	0.26	0.00
Arginine and proline metabolism	77.00	0.42	2.00	0.06	1.00	0.46	0.10
Cyanoamino acid metabolism	16.00	0.09	1.00	0.08	1.00	0.56	0.00
Sulfur metabolism	18.00	0.10	1.00	0.09	1.00	0.57	0.03
Taurine and hypotaurine metabolism	20.00	0.11	1.00	0.10	1.00	0.59	0.00
Selenoamino acid metabolism	22.00	0.12	1.00	0.11	1.00	0.60	0.00
Alanine, aspartate and glutamate metabolism	24.00	0.13	1.00	0.12	1.00	0.61	0.21
Pantothenate and CoA biosynthesis	27.00	0.15	1.00	0.14	1.00	0.63	0.00
beta-Alanine metabolism	28.00	0.15	1.00	0.14	1.00	0.63	0.00
Pentose phosphate pathway	32.00	0.17	1.00	0.16	1.00	0.64	0.00
Vitamin B6 metabolism	32.00	0.17	1.00	0.16	1.00	0.64	0.01
Butanoate metabolism	40.00	0.22	1.00	0.20	1.00	0.73	0.00
Galactose metabolism	41.00	0.22	1.00	0.20	1.00	0.73	0.00
Histidine metabolism	44.00	0.24	1.00	0.21	1.00	0.74	0.14
Fructose and mannose metabolism	48.00	0.26	1.00	0.23	1.00	0.74	0.00
Glycine, serine and threonine metabolism	48.00	0.26	1.00	0.23	1.00	0.74	0.10
Pyrimidine metabolism	60.00	0.32	1.00	0.28	1.00	0.86	0.00
Amino sugar and nucleotide sugar metabolism	88.00	0.48	1.00	0.38	1.00	1.00	0.00
Purine metabolism	92.00	0.50	1.00	0.40	1.00	1.00	0.00
Porphyrin and chlorophyll metabolism	104.00	0.56	1.00	0.44	1.00	1.00	0.00