

Table S1. Clinical biochemical comparison of the three groups.

	Control (n=26)	Normal PCOS (n=26)
age (years)	28.77±3.06	28.46±3.47
Gestation (days)	46.38±4.66	47.46±3.33
BMI (kg/m ²)	21.63±2.04	21.98±1.05
Waist-hip ratio	0.79±0.03	0.81±0.04
E ₂	9.51±0.83	8.94±0.74 ^a
P (ng/ml)	25.28±4.88	20.03±5.23 ^a
β-HCG	4.78±0.52	4.10±0.46 ^a
T(ng/ml)	4.71±0.63	5.85±0.61 ^a
DHEAS(pg/ml)	38.01±8.07	38.40±7.53
AND(nmol/l)	14.88±1.97	21.26±2.50 ^a
SHBG(nmol/l)	26.96±3.18	21.87±3.21 ^a
LDL (ng/dl)	10.11±1.17	10.99±2.72
HDL (pg/ml)	57.27±8.26	47.26±9.54 ^a
TG(nmol/l)	40.39±0.99	41.75±3.61
TC(nmol/l)	15.51±1.71	20.14±1.61 ^a
FPG(mmol/l)	4.72±0.69	4.89±0.92
FINS(Um/l)	10.30±1.48	11.16±1.40
HOMA-IR	2.17±0.51	2.42±0.51

^a p < 0.05 control compared with PCOS.

the data of E₂ and β-HCG after a logarithmic transformation

Table S2. Potential biomarkers identified in positive and negative ESI mode.

metabolite	VIP	Rt (min)	accurate mass	variance	ESI	model	class	pathway
LPC 16:0sn-1	13.4	9.56	496.34	↑	+		lysophosphatidylcholines	lipid metabolism
LPC 16:0sn-2	4.42	9.31	496.34	↑	+		lysophosphatidylcholines	lipid metabolism
LPC 18:0 sn-1	8.08	10.75	524.37	↑	+		lysophosphatidylcholines	lipid metabolism
LPC 18:1 sn-1	4.28	9.98	522.36	↑	+		lysophosphatidylcholines	lipid metabolism
FFA 18:1	11.10	14.57	281.25	↓	-		free fatty acid	lipid metabolism
CarnitineC2:0	5.94	0.75	204.12	↓	+		carnitine	beta oxidation of fatty acids
CarnitineC10:0	3.13	6.17	316.25	↓	+		carnitine	beta oxidation of fatty acids

^a show difference in the PCOS women compared with that in health women.