Supplementary material

Integrated gut microbiota and fecal metabolome analyses of the effect of Lycium barbarum polysaccharide on D-galactose-induced premature ovarian insufficiency

Huili ZHENG[1], Xiaofei LIANG[1], Hongli ZHOU[1], Tong ZHOU[1], Xinhui LIU[1], Jialun DUAN[1], Jinao DUAN*[1], Yue ZHU*[1]

Affiliation

1. Jiangsu Collaborative Innovation Center of Chinese Medicinal Resources Industrialization, National and Local Collaborative Engineering Center of Chinese Medicinal Resources Industrialization and Formulae Innovative Medicine, and Jiangsu Key Laboratory for High Technology Research of TCM Formulae, Nanjing University of Chinese Medicine, Nanjing 210023, China

**** Corresponding author:***

1. Dr. Yue ZHU; E-mail: zhuyue@njucm.edu.cn; Tel: 86-025-8581 1917; Fax: 86-025-8581 1917

2. Dr. Jin-ao DUAN; E-mail: dja@njucm.edu.cn; Tel: 86-025-8581 1917; Fax: 86-025-8581 1917

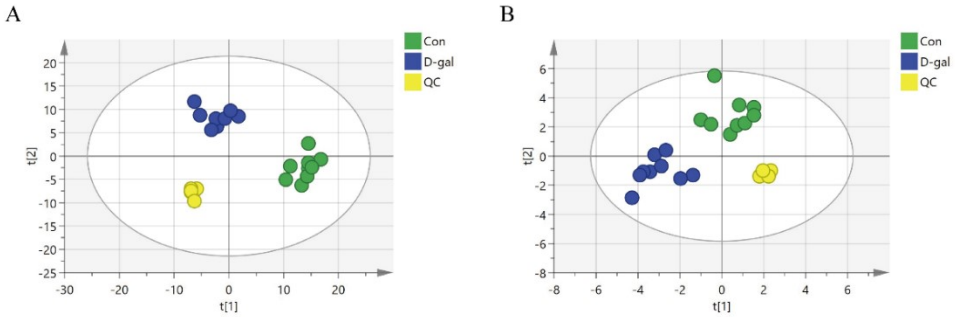

Fig. S1 Quality control samples were clustered on the partial least squares discriminant analysis score plot. (A. ESI+, B. ESI-).

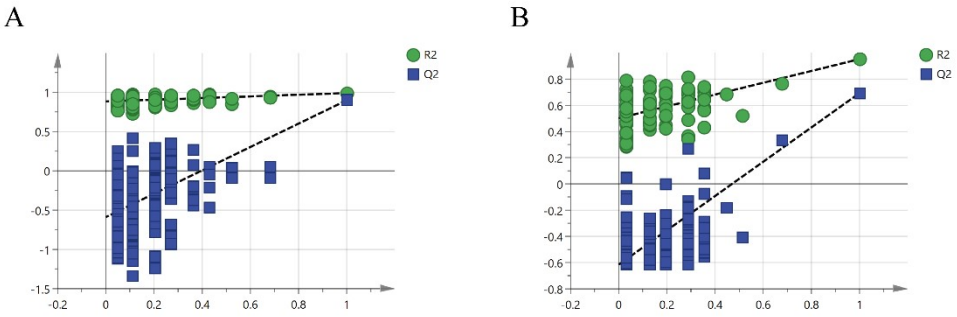

Fig. S2 Permutation test charts for partial least squares discriminant analysis model (A. ESI+, B. ESI-)

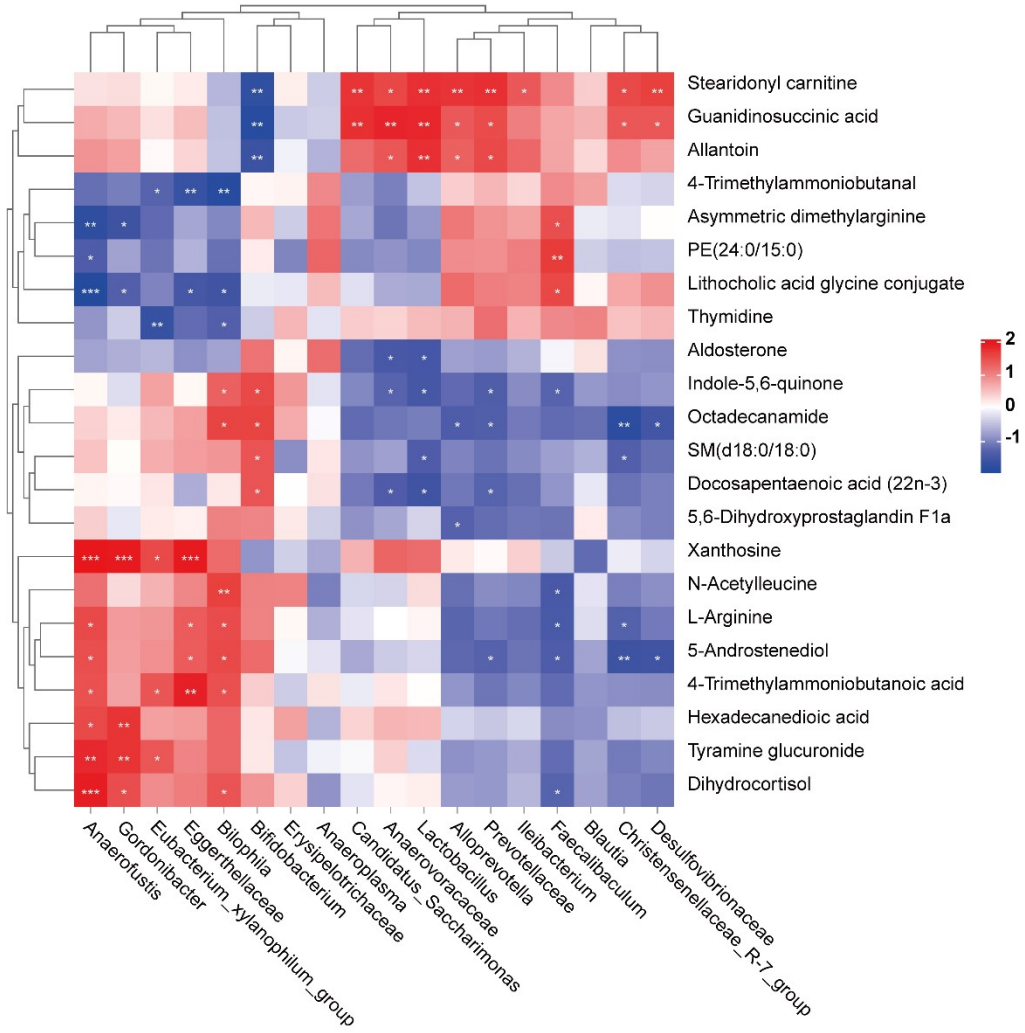

Fig. S3 Correlation analysis between gut microbiota and metabolites. $^{*}P < 0.05$, $^{**}P < 0.01$, $^{***}P < 0.001$.

Table S1 Potential biomarkers identified between the control and model groups in feces.

NO.	RT	m/z	Formula	Common Name	Ion mode	VIP	P	Trend	HMDB
1	0.61	148.1016	Stearidonyl carnitine	$C_{25}H_{41}NO_4$	+	2.01131	0.00023	↓	HMDB0006463
2	0.87	137.0144	Guanidinosuccinic acid	$C_5H_9N_3O_4$	+	1.82788	0.00073	↓	HMDB0003157
3	1.89	377.1283	Tyramine glucuronide	$C_{14}H_{19}NO_7$	+	1.32339	0.00162	↑	HMDB0010328
4	10.24	300.2654	4-Trimethylammoniobutanal	$C_7H_{16}NO$	+	1.27665	0.00133	↓	HMDB0001345
5	10.31	263.2104	Asymmetric dimethylarginine	$C_8H_{18}N_4O_2$	+	1.89021	0.01016	↓	HMDB0001539
6	11.58	279.2066	Lithocholic acid glycine conjugate	$C_{26}H_{43}NO_4$	+	1.09827	0.00073	↓	HMDB0000698
7	11.68	264.2177	PE(24:0/15:0)	$C_{44}H_{88}NO_8P$	+	3.02052	0.00595	↓	HMDB0009714
8	13.13	165.0599	Allantoin	$C_4H_6N_4O_3$	+	1.1265	0.00039	↓	HMDB0000462
9	13.47	443.2547	Aldosterone	$C_{21}H_{28}O_5$	+	1.19573	0.03207	↑	HMDB0000037
10	2.11	162.0242	Xanthosine	$C_{10}H_{12}N_4O_6$	+	1.53473	0.02830	↑	HMDB0000299
11	2.81	295.0731	Indole-5,6-quinone	$C_8H_5NO_2$	+	1.15355	0.00033	↑	HMDB0006779
12	4.01	371.2392	Dihydrocortisol	$C_{21}H_{32}O_5$	+	1.02032	0.00155	↑	HMDB0003259
13	4.34	389.2518	5,6-Dihydroxyprostaglandin F1a	$C_{20}H_{36}O_7$	+	2.30191	0.00335	↑	HMDB0012109
14	4.58	362.307	Octadecanamide	$C_{18}H_{37}NO$	+	1.41082	0.00001	↑	HMDB0034146
15	4.72	390.2591	L-Arginine	$C_6H_{14}N_4O_2$	+	2.2101	0.00120	↑	HMDB0000517
16	4.93	354.2389	5-Androstenediol	$C_{19}H_{30}O_2$	+	2.40933	0.00005	↑	HMDB0003818
17	9.25	313.2513	Docosapentaenoic acid (22n-3)	$C_{22}H_{34}O_2$	+	1.12186	0.00388	↑	HMDB0006528
18	5.66	367.3127	SM(d18:0/18:0)	$C_{41}H_{85}N_2O_6P$	+	1.01497	0.00145	↑	HMDB0012087
19	5.56	388.2422	N-Acetylleucine	$C_8H_{15}NO_3$	+	4.66382	0.00088	↑	HMDB0011756
20	5.34	354.2347	4-Trimethylammoniobutanoic acid	$C_7H_{15}NO_2$	+	4.35259	0.00012	↑	HMDB0001161
21	11.38	303.1562	Thymidine	$C_{10}H_{14}N_2O_5$	−	1.04058	0.03078	↓	HMDB0000273
22	13.12	331.1834	Hexadecanedioic acid	$C_{16}H_{30}O_4$	−	1.03941	0.03405	↑	HMDB0000672

RT: Retention time (min), VIP: variable importance projection

↑ indicates that the compound in the model group is increased compared with the control group, and ↓ indicates that the compound in the model group is decreased compared with the control group.