

Supplementary Material

Table S1 UPLC/Q-TOF MS mobile phase gradient elution procedure for the analysis of serum.

Time (min)	Mobile phase A (%)	Mobile phase B (%)
0~0.5	5	95
0.5~7	5~35	65~95
7~8	35~60	40~65
8~9	60	40
9~9.1	60~5	40~95
9.1~12	5	95

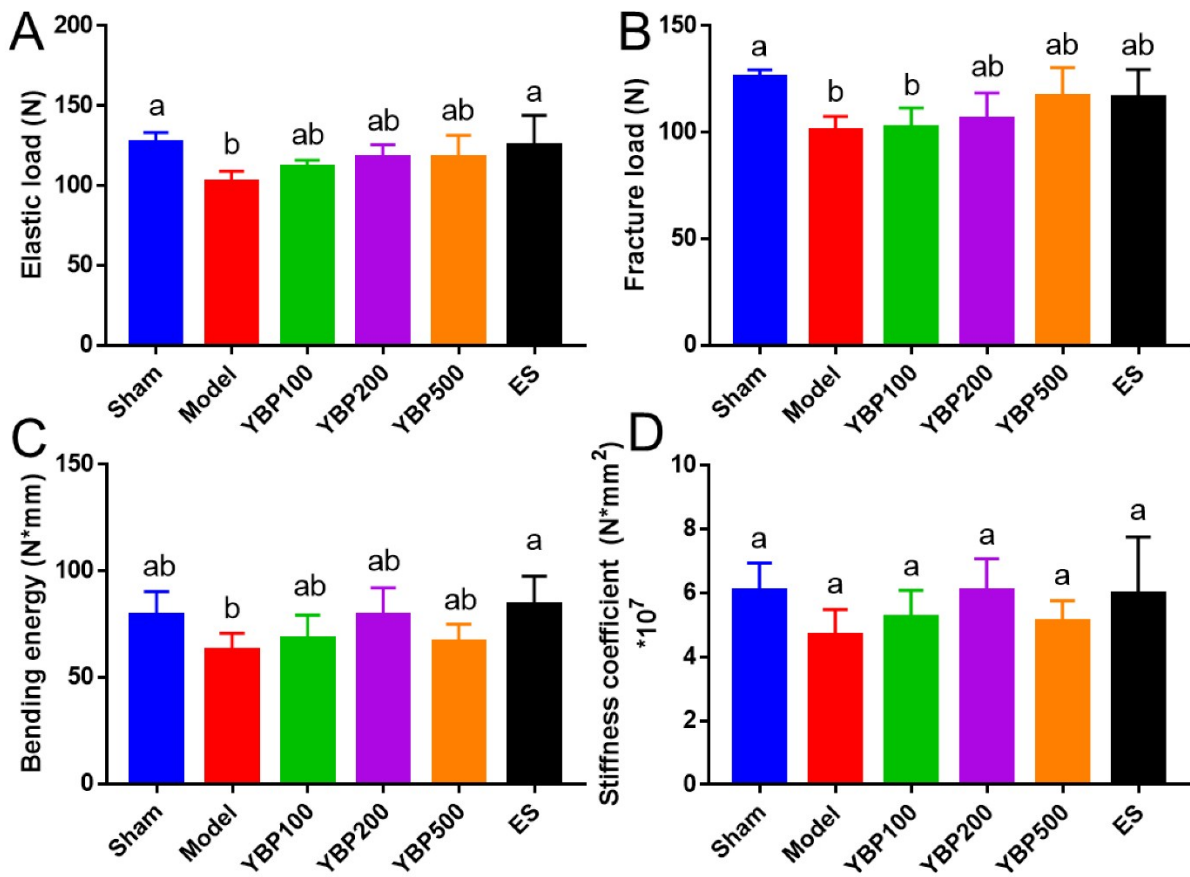


Fig. S1 Bone biomechanical parameters measured by three-point bending test

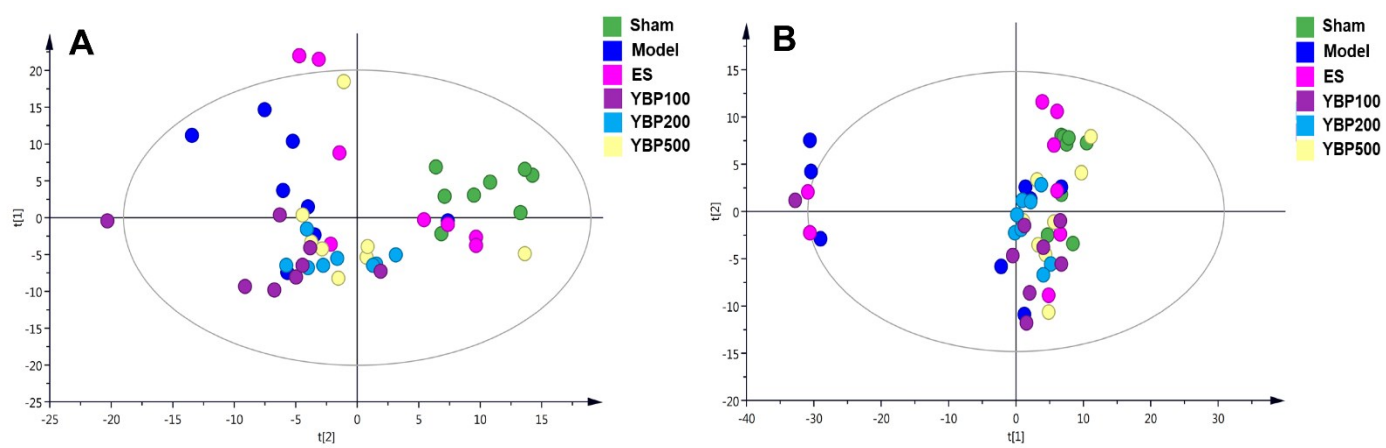


Fig. S2 Metabolite profiling analysis of ovariectomized rats (PCA scores plots, positive mode: A; negative mode: B).

Table S2 Metabolites with significant differences between Sham and Model groups

No.	Adduct	Description	m/z	p-value	VIP	Fold change
1	(M-H)-	DL-lactate	89.0245	0.00813	3.5595	1.26
2	(M-H)-	Creatinine	112.0511	0.03110	1.3381	0.62
3	(M-H)-	Indole	116.0501	0.00776	1.2160	2.27
4	(M-H)-	L-Threonine	118.0510	0.00503	1.3004	1.60
5	(M+H)+	Betaine	118.0846	0.02031	21.1039	0.87
6	(M-H)-	L-Isoleucine	130.0881	0.01228	1.9882	1.25
7	(M+CH ₃ COO)-	Pyruvaldehyde	131.0343	0.04201	1.1723	0.70
8	(M-H)-	L-Lysine	145.0975	0.00122	1.1470	1.47
9	(M+NH ₄)+	L-Pyroglutamic acid	147.0739	0.00998	1.6205	0.87
10	(M-H)-	Vanillin	151.0396	0.00079	1.0624	2.50
11	(M-H ₂ O-H)-	D-Tagatose	161.0452	0.02127	2.7768	0.73
12	(M-H)-	Uric acid	167.0212	0.04694	3.8404	0.57
13	(M+H)+	4-Pyridoxic acid	184.0583	0.02877	1.2893	0.66
14	(M+H)+	Phosphorylcholine	184.0710	0.00000	1.6688	1.67
15	(M-H)-	Indoleacrylic acid	186.0562	0.00244	2.1236	2.85
16	(M+H-H ₂ O)+	DL-Indole-3-lactic acid	188.0690	0.00365	3.8271	1.27
17	(M-H)-	3-Indolepropionic acid	188.0720	0.00808	7.6162	2.30
18	(M-H ₂ O-H)-	3-Hydroxydodecanoic acid	197.1540	0.02615	2.1393	0.40
19	(M-H)-	L-Tryptophan	203.0837	0.00099	5.1567	1.71
20	(M+H)+	Ile-Ala	203.1371	0.00814	1.5707	0.29
21	(M-H)-	Pantothenate	218.1035	0.00848	1.5172	1.81

Table S2 Metabolites with significant differences between YBP500 and Model groups (*Continued*)

No.	Adduct	Description	m/z	p-value	VIP	Fold change
22	(M-H)-	2'-Deoxyuridine	227.0671	0.00105	2.7734	2.42
23	(M+CH ₃ COO)-	D-Mannose	239.0774	0.01477	5.8732	0.54
24	(M-H)-	Cytidine	242.0780	0.03779	1.0261	1.64
25	(M+H)+	Ile-Arg	288.2020	0.01520	1.2924	0.57
26	(M+NH ₄)+	Linoleic acid	298.2742	0.03319	2.0156	1.43
27	(M-H)-	12(R)-HETE	319.2288	0.01011	22.6052	2.78
28	(M+H)+	Erucamide	338.3415	0.02378	2.9482	4.22
29	(M+NH ₄)+	(4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-Docosahexaenoic acid	346.2748	0.00011	6.4181	1.90
30	(2M-H)-	D-Fructose	359.1194	0.02795	4.6847	0.52
31	(M-H)-	Sphingosine-1-phosphate	378.2411	0.00500	1.2704	1.69
32	(M+H)+	L-Palmitoylcarnitine	400.3429	0.00437	2.4388	1.66
33	(M+H)+	1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	454.2948	0.00226	3.7479	2.31
34	(M+Na-2H)-	1-Oleoyl-sn-glycerol 3-phosphate	457.2355	0.00000	2.0786	4.15
35	(M+H)+	1-Myristoyl-sn-glycero-3-phosphocholine	468.3099	0.02470	2.4038	1.57
36	(M+H)+	1-Palmitoyl-sn-glycero-3-phosphocholine	496.3402	0.02518	1.1734	1.70
37	(M+H-H ₂ O)+	1-Stearoyl-sn-glycerol 3-phosphocholine	506.3611	0.00001	2.0645	1.64
38	(M+H)+	1-Oleoyl-sn-glycero-3-phosphocholine	522.3572	0.00003	13.3470	1.65
39	(M+H)+	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine	524.3744	0.00000	32.9755	1.56
40	M+	1-O-(cis-9-Octadecenyl)-2-O-acetyl-sn-glycero-3-phosphocholine	550.3880	0.00058	2.6601	1.77
41	(M-H+2Na)+	1,2-dioleoyl-sn-glycero-3-phosphatidylcholine	830.5775	0.00802	5.1875	1.81
42	(M-2H+3Na)+	1-Stearoyl-2-oleoyl-sn-glycerol 3-phosphocholine (SOPC)	854.5784	0.00646	2.6400	1.73

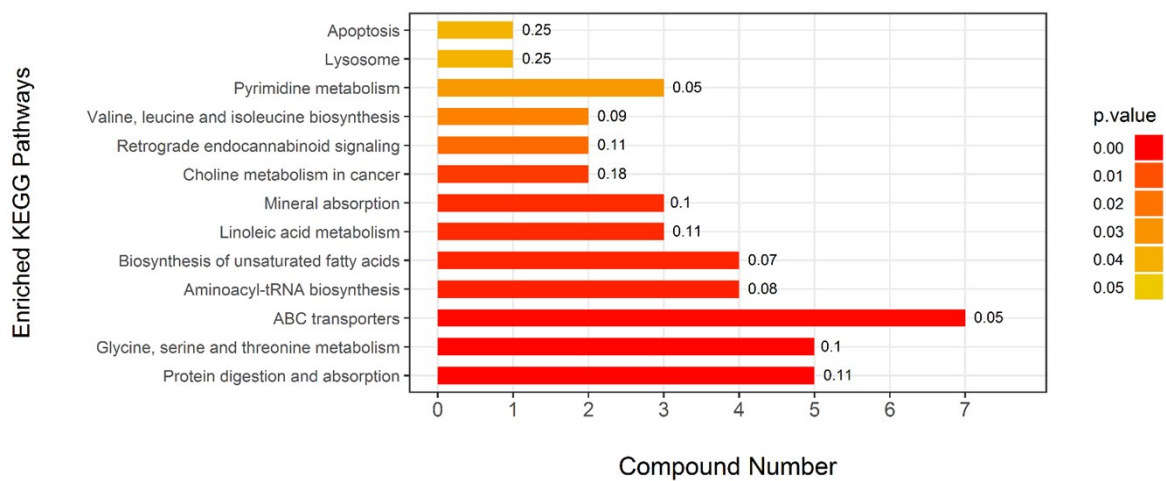


Fig. S3 The enriched KEGG pathways of the metabolites between Sham and Model.