iScience, Volume *25*

Supplemental information

Low-density lipoprotein receptor genotypes modify the sera metabolome of patients with homozygous familial hypercholesterolemia

Zhiyong Du, Fan Li, Linyi Li, Yu Wang, Jianping Li, Ya Yang, Long Jiang, Luya Wang, and Yanwen Qin

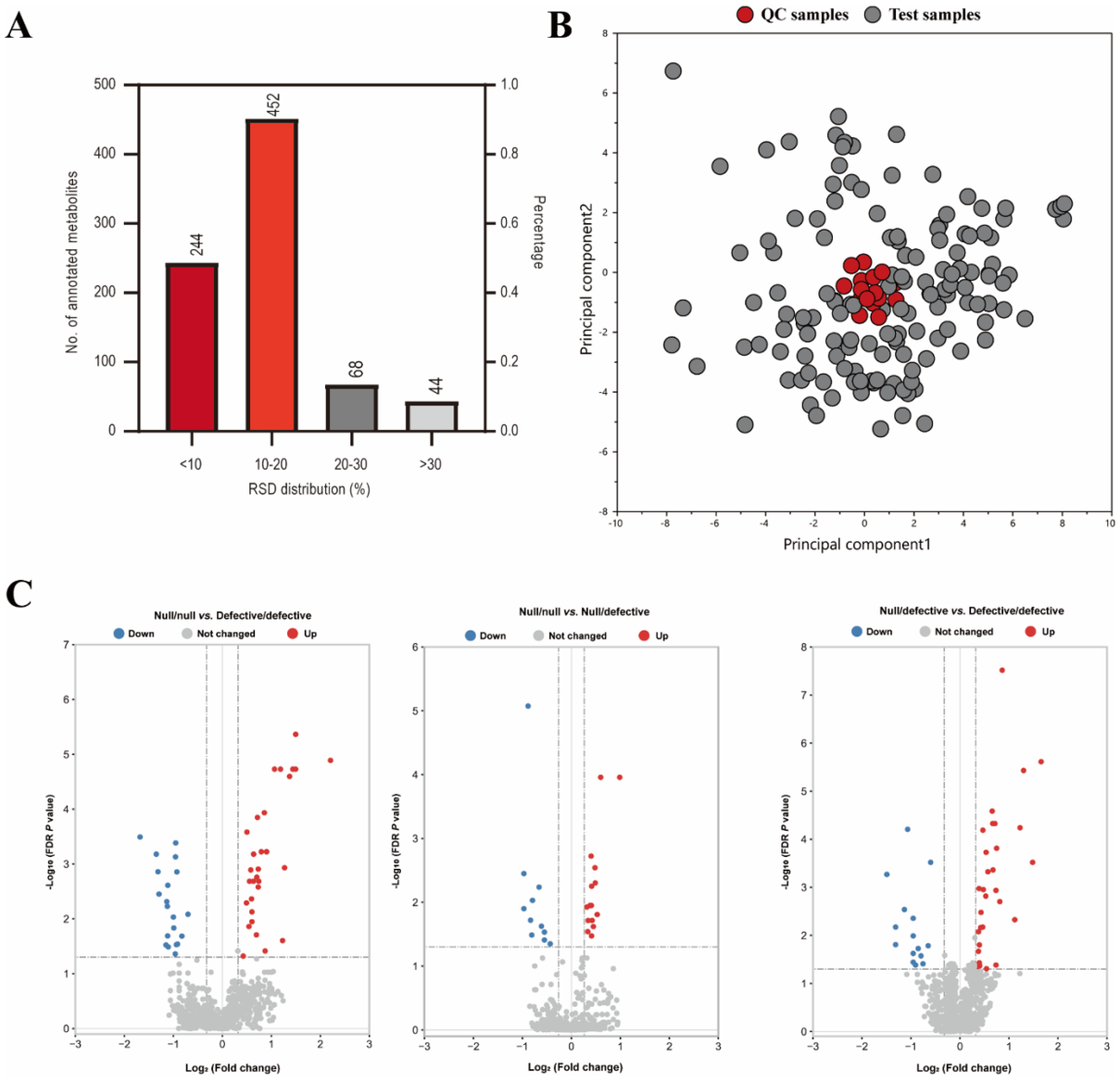

Figure S1. Pattern analysis of metabolomic data, Related to Figures 1 and 2. (A) Stability of analytical methods based on QC samples. (B) PCA scores plot of test samples and QC samples; each point represents an individual serum sample. (C) Volcano plots of each metabolite variation in pairwise comparisons of defective/defective, null/defective, and null/null groups; the dashed lines indicate the threshold for the significant differences.

Table S2 Differentiated metabolites in the serum samples from null/null, null/defective, and defective/defective groups, Related to Figure 2

Metabolites	NN versus DD			NN versus ND			ND versus DD		
	FC	P value	FDR	FC	P value	FDR	FC	P value	FDR
3-Indoxyl sulfate	0.57204	0.003088	0.005318	0.79261	0.43988	0.54545	0.72171	0.0079176	0.015835
Betaine	1.7344	1.01E-05	4.82E-05	1.17	0.21726	0.33676	1.4825	0.00002034	9.0076E-05
CE 16:0	1.5521	6.17E-05	0.000174	1.1538	0.042734	0.10598	1.3452	0.00048258	0.00136
CE 16:1	1.4575	0.000537	0.001189	1.2458	0.025289	0.074664	1.17	0.078903	0.10871
CE 18:0	1.7766	9.48E-08	1.04E-06	1.3267	0.00181	0.011224	1.3391	0.0014104	0.0034977
CE 18:1	1.5562	1.29E-05	5.70E-05	1.119	0.18216	0.2972	1.3907	9.8485E-05	0.00035918
Cholesterol	1.4959	3.00E-05	0.000109	1.2676	0.005293	0.019302	1.1801	0.025034	0.044315
Cholic acid	1.8719	9.64E-06	4.82E-05	1.4414	0.003511	0.015547	1.2986	0.0062322	0.01288
Docosahexaenoic acid	0.61157	1.97E-05	8.15E-05	0.58399	1.32E-07	8.17E-06	1.0472	0.22852	0.28337
Glutamine	0.62561	3.44E-05	0.000118	0.77265	0.000672	0.005607	0.8097	0.034576	0.054302
Glycocholic acid	1.6322	8.44E-08	1.04E-06	1.246	0.002292	0.011844	1.3099	8.8228E-05	0.00034188
Histidine	0.75347	0.000348	0.000829	0.93304	0.39385	0.51955	0.80754	2.6381E-05	0.00010904
Hypoxanthine	2.1149	1.00E-07	1.04E-06	1.1647	0.02663	0.075049	1.8158	3.9567E-11	2.4531E-09
Linoleic acid	1.6283	4.51E-05	0.000147	1.3305	0.010837	0.033594	1.2238	0.017106	0.032138
Lysine	0.67142	0.000883	0.001824	1.0994	0.19914	0.31659	0.61071	4.5524E-08	1.4113E-06
LysoPC 16:0	1.4682	5.90E-05	0.000174	1.1297	0.066401	0.14196	1.2996	0.0017557	0.0041866

LysoPC 18:0	1.4069	0.000166	0.00043	1.3036	0.001691	0.011224	1.0793	0.3508	0.3945
LysoPC 18:1	1.8666	1.01E-05	4.82E-05	1.1707	0.1486	0.26324	1.5945	1.8052E-05	8.6096E-05
LysoPC 18:2	1.6738	6.17E-05	0.000174	1.365	0.006968	0.023999	1.2262	0.029474	0.049389
LysoPC O-18:1	1.8115	1.21E-06	9.35E-06	1.0796	0.13501	0.25861	1.6779	2.1982E-06	1.5143E-05
LysoPC O-18:2	2.2009	1.28E-09	7.95E-08	1.3964	0.000232	0.002876	1.5761	1.0128E-07	2.0931E-06
LysoPC 16:1	1.5114	0.000135	0.000363	1.1492	0.079181	0.15836	1.3151	0.004059	0.0089879
LysoPA 16:0	2.3742	0.006364	0.009864	0.85052	0.55396	0.64803	2.7915	8.4868E-06	4.6073E-05
LysoPE O-18:2	1.5205	0.000424	0.000974	0.95763	0.77881	0.8265	1.5878	3.1031E-07	4.5543E-06
LysoPI 18:0	2.0543	0.006997	0.01058	0.87929	0.17889	0.2972	2.3364	5.7296E-07	5.9206E-06
LysoPI 18:1	1.5204	0.000252	0.000624	1.0515	0.27422	0.39386	1.446	3.8871E-06	0.0000241
Methionine	0.68545	0.002187	0.003988	0.81222	0.059313	0.1362	0.84391	0.077108	0.10871
Palmitic acid	1.6187	0.000788	0.001685	1.1752	0.1458	0.26324	1.3774	0.00131	0.0033841
Palmitoyl-carnitine	1.3437	0.002602	0.004609	1.2617	0.008841	0.02885	1.065	0.070257	0.10371
Phenylalanine	2.1981	9.48E-08	1.04E-06	1.342	0.004974	0.019273	1.6379	3.6728E-07	4.5543E-06
Purine	1.4156	3.40E-06	2.11E-05	1.3223	0.000122	0.001892	1.0706	0.1304	0.17202
Retinoic acid	2.0188	1.59E-07	1.41E-06	1.4026	0.000481	0.004975	1.4393	0.00015852	0.00051727
Serine	1.8317	0.0019	0.003569	1.1018	0.78651	0.8265	1.6624	0.00010986	0.00037841
Sphingosine	1.246	0.0019	0.003569	1.1604	0.030255	0.081557	1.0738	0.020451	0.037293
Stearoyl-carnitine	1.6434	1.65E-06	1.14E-05	1.3326	0.000724	0.005607	1.2332	0.0026898	0.0061765

TAG 52:2	1.6238	0.003194	0.005353	1.3986	0.052865	0.12606	1.161	0.10098	0.1361
TAG 52:3	1.328	0.00722	0.010658	1.5142	5.52E-06	0.000151	0.87702	0.4175	0.4463
TAG 54:2	4.6173	3.94E-08	1.04E-06	1.9819	7.33E-06	0.000151	2.3297	0.025731	0.044315
TAG 54:3	1.6628	2.73E-05	0.000106	1.204	0.063486	0.14058	1.3811	8.4066E-07	6.5151E-06
Taurine	0.69793	0.003535	0.005767	1.0578	0.43988	0.54545	0.65982	8.9173E-06	4.6073E-05
Taurocholic acid	2.3442	0.001099	0.002199	1.3355	0.28312	0.39386	1.7553	0.00022658	0.00070238

Two-tailed Student's *t* test or Mann Whitney *U* test were used for each comparison. NN = null/null, ND = null/defective, DD = defective/defective, FC = fold changes, FDR = false discovery rate P value, CE = cholesterol esters, TAG = triacylglycerides, LPI = lysophosphatidylinositol, LysoPC = lysophosphocholines, LysoPC O = alkyl LysoPC, LysoPE = lysophosphoethanolamines, LysoPE O = alkyl LysoPE, LysoPA = lysophosphatidic acid.