Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Summary of potential lipids biomarkers of CHD and SalB therapeutic action by UPLC/MS analysis

No.	Rt(min)	Ion Form	Chenmical Formula	m/z	Error	Proposed Compound	Trend in CHD Model	HMDB Code	Geniposide Regulation	Data significance compared with CHD model
1	0.47	M-H	C61H112O5	923.8351	-9.3174	TG(20:0/20:4/o-18:0)	up	HMDB45996	√	##
2	1.09	M+H	C46H82NO8P	808.5890	4.8498	PC(20:4/18:1)	low	HMDB08433	√	##
3	2.17	M+H	C46H82NO8P	808.5890	4.8498	PC(18:3/20:2)	up	HMDB08177	√	##
4	2.32	M+H	C39H73O8P	701.5082	-4.8308	PA(18:0/18:2)	up	HMDB07861	√	##
5	2.65	M-H	C23H44NO7P	476.2794	3.8052	LysoPE(18:2/0:0)	low	HMDB11507	√	#
6	2.81	M-H	C55H90O6	845.6704	4.5937	TG(14:1/18:4/20:3)	up	HMDB48281		
7	3.07	M-H	C45H91N2O6P	785.6510	-4.0066	SM(d18:0/22:1)	low	HMDB12092	√	##
8	3.48	M-H	C18H38NO5P	378.2450	9.57E-08	Sphingosine-1-phosphate	low	HMDB00277	√	##
9	3.66	M-H	C27H44NO7P	524.2800	0.0545	PE(22:6/0:0)	low	HMDB0011526	√	#
10	3.97	M-H	C25H44NO7P	500.2800	0.1107	LysoPE(20:4/0:0)	up	HMDB11517	√	#
11	4.62	M+H	C18H39NO2	302.3066	4.1583	Sphinganine	up	HMDB00269	√	##
12	5.10	M-H	C36H73NO3	566.5516	0.0432	Cer(d18:0/18:0)	up	HMDB0011761	√	##
13	5.23	M-H	C42H76NO10P	784.5170	0.4862	PS(18:0/18:3)	low	HMDB12381		
14	5.85	M+H	C28H54NO7P	548.3723	2.2723	LysoPC(20:2)	up	HMDB10392		
15	6.24	M-H	C34H64NO10P	676.4191	-0.6011	PS(14:0/14:1)	low	HMDB12331	√	##
16	6.49	M+H	C20H32O5	353.2353	3.3300	Prostaglandin E2	up	HMDB01220	√	#
17	6.86	M+H	C20H32O2	327.23	-2.4511	Arachidonic acid	up	HMDB01043	√	##
18	6.99	M+H	C42H84NO8P	762.5971	-4.7685	PC (18:0/16:0)	up	HMDB08034	√	##
19	7.24	M+H	C25H52NO7P	510.3532	-4.376	LysoPC(17:0)	up	HMDB12108	√	##
20	7.72	M-H	C47H88NO8P	824.6235	7.2787	PE(22:2/20:1)	low	HMDB09560	√	##
21	7.93	M+H	C48H82NO8P	832.5871	2.3712	PC(20:3/20:4)	up	HMDB08410	√	##
22	8.23	M+H	C46H93N2O6P	801.6805	-4.8802	SM(d18:1/23:0)	up	HMDB12105		
23	8.47	M+H	C58H98O6	891.7355	-9.0719	TG(15:0/22:6/18:1)	up	HMDB43781	√	#
24	8.75	M-H	C41H74NO7P	722.5122	-1.1214	PE(20:4/P-16:0)	low	HMDB09411	√	#
25	9.11	M+H	C44H80NO10P	814.5640	6.1539	PS(20:3/18:0)	low	HMDB12422	√	#
26	9.68	M+H	C27H46O4S	467.3224	0.00161	Cholesterol sulfate	up	HMDB00653	√	#

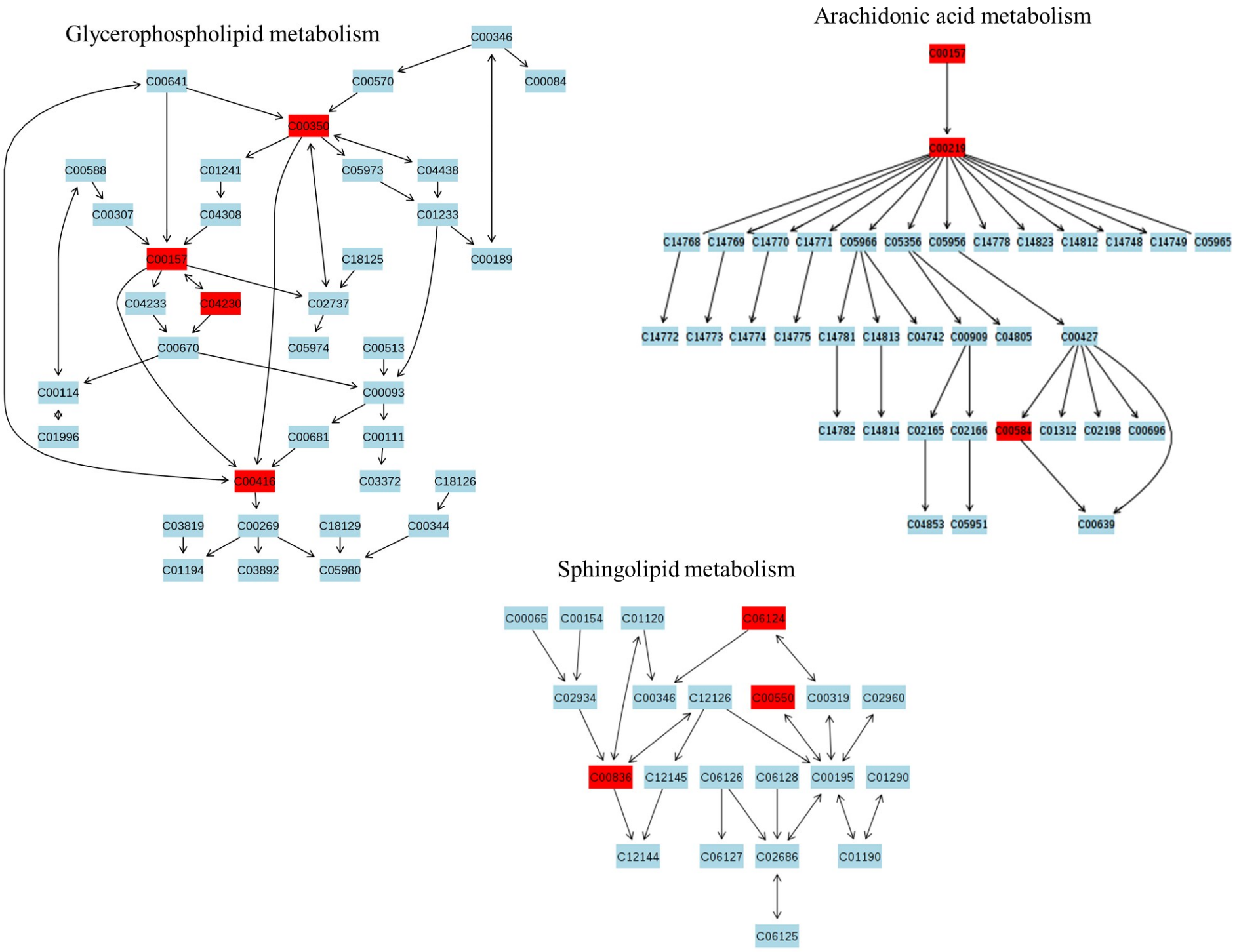

Figure 1S The KEGG pathway of glycerophospholipid metabolism, sphingolipid metabolism and arachidonic acid metabolism.

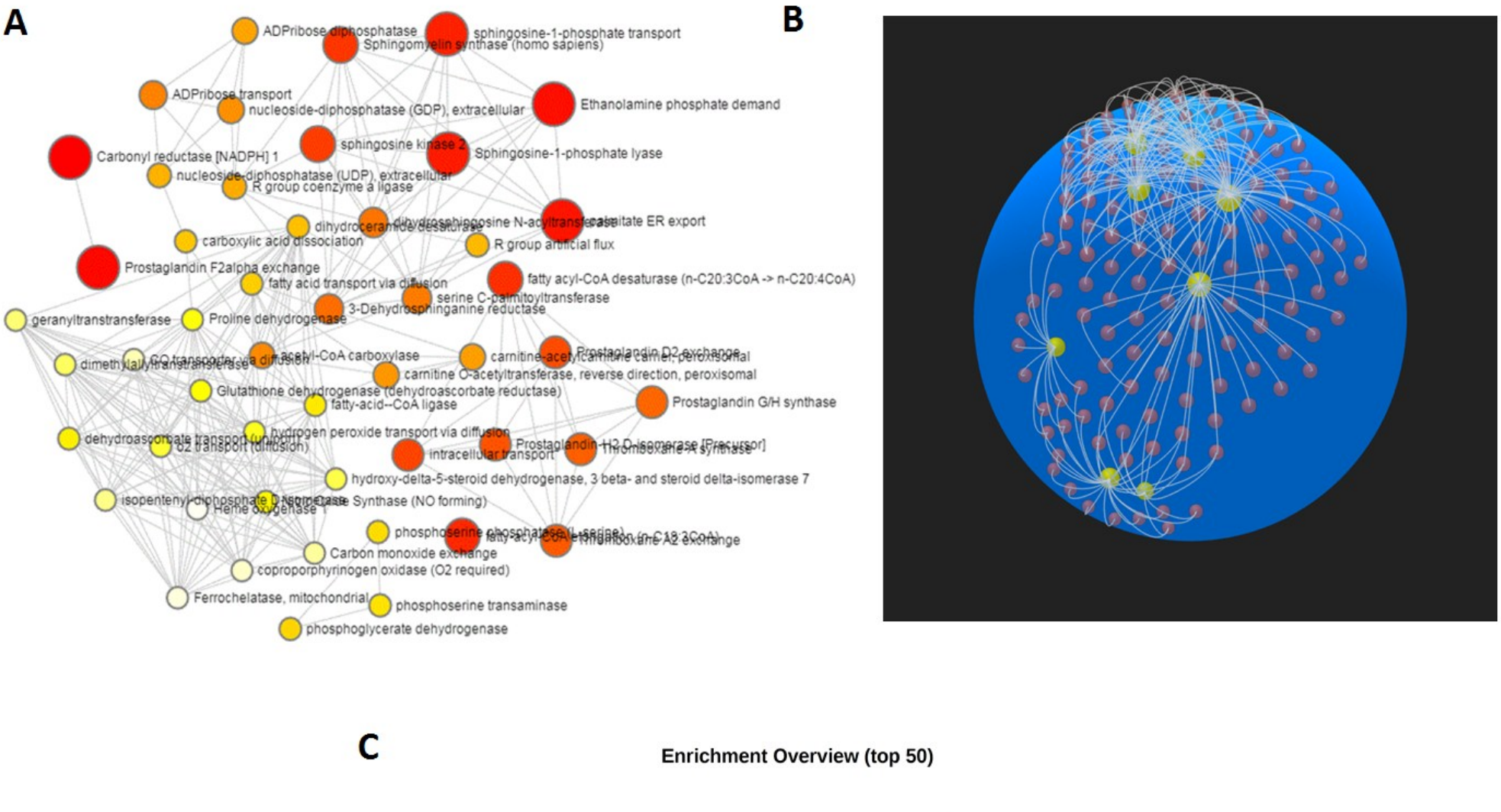

Figure S2 The result of enrichment and network analysis of lipdis metabolites. (A) the enzymes activity affects Sal B pharmacodynamic effects on CHD predicted by genome-scale network model of human metabolism. (B) the relationship between eight lipids affected by Sal B and gene, including arachidonate, phosphatidylcholine, phosphatidylethanolamine, phosphatidate, 1-Acyl-sn-glycero-3-phosphocholine, sphinganine, sphingomyelin, sphingosine 1-phosphate. (C) the reslut of single nucleotide polymorphisms (SNPs) loci of these detected lipids metabolites based on their associations .