| No. | Rt(min) | Ion Form | Chemical 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 | -4.8208   | PA(18:0/18:2)  | up    | HMDB07861  |                        | #                                       |
| 5   | 2.65    | M+H     | C32H44NO8P      | 476.2794 | 3.8052    | LysoPE(18:2/0:0) | low   | HMDB11507  |                        | #                                       |
| 6   | 2.81    | M+H     | C35H90O6        | 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     | C28H54NO7P      | 548.3723 | 2.2723    | LysoPC(20:2)   | up    | HMDB10392  |                        | #                                       |
| 14  | 5.85    | M+H     | C32H44NO10P     | 676.4191 | -0.6011   | PS(14:0/14:1)  | low   | HMDB12331  |                        | #                                       |
| 15  | 6.24    | M+H     | C34H64NO10P     | 535.2353 | 3.3300    | Prostaglandin E2 | up    | HMDB01220  |                        | #                                       |
| 16  | 6.49    | M+H     | C20H32O2        | 327.2327 | -2.4511   | Arachidonic acid | up    | HMDB01043  |                        | #                                       |
| 17  | 6.86    | M+H     | C20H32O2        | 327.2327 | -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     | C46H82NO6P      | 801.6905 | 4.8802    | Sm(d18:1/23:0) | up    | HMDB12105  |                        | #                                       |
| 23  | 8.47    | M+H     | C58H90O6        | 891.7355 | -9.0199   | TG(15:0/22:6/18:1) | up    | HMDB43781  |                        | #                                       |
| 24  | 8.75    | M+H     | C41H74NO7P      | 722.5122 | -1.1214   | PE(20:4/16:0)  | 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 lipids 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, phosphatidylecholine, phosphatidylethanolamine, phosphatidate, 1-Acyl-sn-glycero-3-phosphocholine, sphinganine, sphingomyelin, sphingosine 1-phosphate. (C) the result of single nucleotide polymorphisms (SNPs) loci of these detected lipids metabolites based on their associations.