**Table S4: The detail information of 23 metabolites in metabolomic fingerprint associated with chronic DILI.**

| No. | Scan mode | MZ | RT | Name | Formula | Chronic DILI vs Acute DILI |
| --- | --- | --- | --- | --- | --- | --- |
| AUC | FC | P |
| 1 | ESI+ | 1086.425 | 11.61 | Docosadienoyl-CoA | C43H76N7O17P3S | 0.82 | 4.63 | 2.30E-07 |
| 2 | ESI+ | 370.1656 | 9.73 | PC(3:0/3:0) | C21H23NO5 | 0.82 | 0.22 | 9.78E-05 |
| 3 | ESI+ | 369.1635 | 8.75 | Dehydroepiandrosterone sulfate | C19H28O5S | 0.81 | 0.37 | 1.22E-06 |
| 4 | ESI+ | 357.2622 | 11.66 | Prostaglandin F1a | C20H36O5 | 0.79 | 8.13 | 1.82E-06 |
| 5 | ESI+ | 881.7798 | 11.55 | TG(16:1/18:0/20:4) | C57H100O6 | 0.79 | 2.14 | 9.08E-04 |
| 6 | ESI- | 528.2621 | 4.7 | Glycochenodeoxycholate-3-sulfate | C26H43NO8S | 0.78 | 0.18 | 3.08E-05 |
| 7 | ESI+ | 882.2004 | 11.54 | Hydroxyhexanoyl-CoA | C27H46N7O18P3S | 0.77 | 2.00 | 5.61E-06 |
| 8 | ESI- | 450.3206 | 6.49 | Glyochenodeoxycholic acid | C26H43NO5 | 0.76 | 4.77 | 7.05E-07 |
| 9 | ESI+ | 267.0758 | 9.46 | Monoglyceride citrate | C9H14O9 | 0.76 | 3.47 | 4.53E-03 |
| 10 | ESI+ | 302.3038 | 13.38 | Sphinganine | C18H39NO2 | 0.75 | 2.80 | 1.44E-04 |
| 11 | ESI+ | 575.2308 | 9.32 | Tetrahydrofolyl-[Glu] | C24H30N8O9 | 0.75 | 0.21 | 5.46E-07 |
| 12 | ESI+ | 183.0855 | 11.43 | Galactitol | C6H14O6 | 0.75 | 0.05 | 4.77E-05 |
| 13 | ESI+ | 514.2811 | 8.51 | Taurocholic acid | C26H45NO7S | 0.75 | 0.03 | 1.09E-07 |
| 14 | ESI+ | 276.1762 | 13.09 | Hydroxyhexanoycarnitine | C20H21N | 0.74 | 2.5 | 9.45E-06 |
| 15 | ESI+ | 829.695 | 10.04 | SM(d18:0/24:1(15Z)(OH)) | C48H98N2O6P | 0.74 | 2.52 | 6.88E-05 |
| 16 | ESI- | 854.3734 | 4.44 | CDP-DG(a-13:0/i-12:0) | C37H67N3O15P2 | 0.74 | 0.25 | 2.18E-04 |
| 17 | ESI- | 583.2603 | 5.76 | Bilirubin | C33H36N4O6 | 0.73 | 0.13 | 3.55E-04 |
| 18 | ESI+ | 197.0606 | 10.81 | Galactonic acid | C6H12O7 | 0.73 | 4.94 | 1.59E-05 |
| 19 | ESI+ | 176.0679 | 1.36 | Guanidinosuccinic acid | C5H9N3O4 | 0.73 | 2.56 | 1.35E-06 |
| 20 | ESI+ | 165.092 | 13.66 | 2,4-Decadiynoic acid | C10H12O2 | 0.73 | 4.35 | 8.39E-03 |
| 21 | ESI+ | 355.1513 | 11.14 | S-Adenosylmethioninamine | C14H23N6O3S | 0.73 | 0.40 | 7.01E-04 |
| 22 | ESI+ | 761.2875 | 8.66 | Bilirubin glucuronide | C39H44N4O12 | 0.73 | 3.66 | 2.00E-04 |
| 23 | ESI+ | 175.025 | 3.2 | Cis-Aconitic acid | C6H6O6 | 0.72 | 2.04 | 3.22E-05 |