Table S1. The CE, CXP, Q1, Q3 and time for each bile acid

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bile acid | Retention time(min) | Q1 Mass (m/z) | Q3 Mass(m/z) | Cone(V) | Collision(V) |
| TUDCA | 1.17  | 514.3 | 80.0  | 30 | 60 |
| TCA | 1.19  | 514.3 | 80.0  | 30 | 60 |
| GCA | 1.52  | 464.3 | 74.0  | 30 | 35 |
| GUDCA | 1.54  | 448.3 | 74.0  | 30 | 35 |
| TCDCA | 1.67  | 514.3 | 80.0  | 30 | 60 |
| TDCA | 1.82  | 498.3 | 80.0  | 30 | 60 |
| GCDCA | 2.30  | 448.3 | 74.0  | 30 | 35 |
| CA | 2.47  | 407.3 | 407.3  | 30 | 20 |
| GDCA | 2.48  | 448.3 | 74.0  | 30 | 32 |
| TLCA | 2.55  | 482.3 | 80.0  | 30 | 58 |
| UDCA | 2.60  | 391.2 | 391.2  | 30 | 30 |
| CDCA | 3.59  | 391.2 | 391.2  | 30 | 20 |
| GLCA | 3.61  | 432.2 | 74.0  | 30 | 35 |
| DCA | 3.75  | 391.2 | 391.2  | 30 | 20 |
| LCA | 4.62  | 375.3 | 375.3  | 30 | 20 |