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

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| --- | --- | --- | --- | --- | --- |
| 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 |