**Table S1.** Demonstration of elution gradients for mobile phases in positive and negative ion mode.

|  |  |
| --- | --- |
| Positive Ion Model | Negative Ion Mode |
| Time (min) | Flow rate (mL/min) | A (%) | B (%) | Time (min) | Flow rate (mL/min) | A (%) | B (%) |
| 0 | 0.4 | 100 | 0 | 0 | 0.4 | 100 | 0 |
| 3 | 0.4 | 80 | 20 | 1.5 | 0.4 | 95 | 5 |
| 4.5 | 0.4 | 65 | 35 | 2 | 0.4 | 90 | 10 |
| 5 | 0.4 | 0 | 100 | 4.5 | 0.4 | 70 | 30 |
| 6.3 | 0.4 | 0 | 100 | 5 | 0.4 | 0 | 100 |
| 6.4 | 0.4 | 100 | 0 | 6.3 | 0.4 | 0 | 100 |
| 8 | 0.4 | 100 | 0 | 6.4 | 0.4 | 100 | 0 |
| 8 | 0.4 | 100 | 0 |