**S1 Table** LC elution gradient in ESI-positive and -negative modes

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Mode | Mobile phase /% | Time /min | | | | | |
| 0 | 1 | 10 | 19 | 20 | 23 |
| ESI-Positive | A (10 mM aqueous ammonium acetate) | 4 | 4 | 2 | 2 | 4 | 4 |
| B (isopropanol) | 6 | 6 | 83 | 83 | 6 | 6 |
| C (methanol) | 90 | 90 | 15 | 15 | 90 | 90 |
| ESI-Negative | A (10 mM aqueous ammonium acetate) | 25 | 5 | 5 | 0 | 25 | 25 |
| B (isopropanol) | 40 | 60 | 60 | 65 | 40 | 40 |
| C (methanol) | 35 | 35 | 35 | 35 | 35 | 35 |