|  |  |  |
| --- | --- | --- |
| **Table S3.** | **MS Parameters for Q Exactive** |  |
|  | Top 5 |  |
| Polarity | Positive | Negative |
|  | Full Scan | Full Scan |
| Resolution | 70000 | 70000 |
| AGC | 1.00E+06 | 1.00E+06 |
| Maximum IT(ms) | 50 | 50 |
| Scan range (m/z) | 300-1800 | 300-1800 |
|  | TopN (ddMS2) | TopN (ddMS2) |
|  | 5 | 5 |
| Resolution | 17500 | 17500 |
| AGC | 1.00E+05 | 1.00E+05 |
| Maximum IT(ms) | 117 | 117 |
| Isolation window (m/z) | 1 | 1 |
| NCE | 25,30 | 25,30 |
| Dynamic exclusion (s) | 20 | 20 |
| Minimum AGC | 2.00E+02 | 2.00E+02 |
|  |  |  |
| AGC | Automatic gain control |  |
| IT | Injection time |  |
| NCE | Normalized collision energy |  |