S4 Table

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| DataFrom | Score | MW | Compound Key | PPM Error | Theoretical MW | NumCharges | Total Volume |
| Replicate 1 | 0.14 | 4731.0948 | [8,8,1,22,0] | 0.35 | 4731.0964 | 2 | 121596 |
| 0.14 | 3595.9691 | [8,8,1,6,1] | 3.28 | 3595.9573 | 1 | 375 |
| 0.19 | 5091.8954 | [9,9,1,24,0] | 0.61 | 5091.8986 | 5 | 680683 |
| 0.51 | 5376.1808 | [9,9,1,25,0] | 1.28 | 5376.1740 | 4 | 8930501 |
| 0.14 | 5316.0187 | [9,9,1,25,1] | 1.22 | 5316.0252 | 2 | 127367 |
|  |  |  |  |  |  |  |  |
| Replicate 2 | 0.16 | 4765.1480 | [8,8,1,22,0] | 0.32 | 4765.1495 | 2 | 88139 |
| 0.12 | 3459.7410 | [8,8,1,6,1] | 1.11 | 3459.7449 | 1 | 357 |
| 0.17 | 5091.8956 | [9,9,1,24,0] | 0.59 | 5091.8986 | 5 | 1455128 |
| 0.36 | 5376.1794 | [9,9,1,25,0] | 1.01 | 5376.1740 | 4 | 7721203 |
| 0.14 | 5350.0597 | [9,9,1,25,1] | 3.48 | 5350.0783 | 3 | 226158 |
|  |  |  |  |  |  |  |  |
| Replicate 3 | 0.14 | 4594.8826 | [8,8,1,22,0] | 0.31 | 4594.8840 | 2 | 54087 |
| 0.13 | 3357.5691 | [8,8,1,6,1] | 4.90 | 3357.5856 | 1 | 506 |
| 0.18 | 5091.8952 | [9,9,1,24,0] | 0.67 | 5091.8986 | 4 | 863846 |
| 0.36 | 5342.1420 | [9,9,1,25,0] | 3.95 | 5342.1209 | 4 | 9688604 |
| 0.14 | 5418.1815 | [9,9,1,25,1] | 0.56 | 5418.1845 | 2 | 27302 |