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 |