S2 Table

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| DataFrom | Score | MW | Compound Key | PPM Error | Theoretical MW | NumCharges | Total Volume |
| Replicate 1 | 0.18  | 3989.2840  | [8,8,1,14,0] | 0.34  | 3989.2826  | 1 | 668826 |
| 0.17  | 4434.9659  | [8,8,1,20,0] | 1.02  | 4434.9704  | 6 | 641929 |
| 0.17  | 4514.9332  | [8,8,1,21,0] | 1.32  | 4514.9272  | 6 | 2212394 |
| 0.14  | 4659.1131  | [8,8,1,21,1] | 3.44  | 4659.0971  | 1 | 1382 |
| 0.60  | 4594.8913  | [8,8,1,22,0] | 1.59  | 4594.8840  | 8 | 17739238 |
| 0.16  | 4773.1126  | [8,8,1,22,1] | 1.18  | 4773.1070  | 3 | 3732677 |
| 0.14  | 5268.5989  | [8,8,1,30,0] | 1.38  | 5268.5916  | 1 | 458 |
| 0.14  | 5296.2155  | [9,9,1,24,0] | 0.31  | 5296.2171  | 1 | 444 |
|  |  |  |  |  |  |  |  |
| Replicate 2 | 0.15  | 4006.3090  | [8,8,1,14,0] | 0.04  | 4006.3092  | 1 | 14127 |
| 0.15  | 4434.9571  | [8,8,1,20,0] | 3.00  | 4434.9704  | 6 | 531513 |
| 0.17  | 4685.2120  | [8,8,1,21,0] | 4.11  | 4685.1927  | 2 | 3758087 |
| 0.13  | 4625.0664  | [8,8,1,21,1] | 4.84  | 4625.0440  | 1 | 3206 |
| 0.58  | 4594.8923  | [8,8,1,22,0] | 1.81  | 4594.8840  | 8 | 20140278 |
| 0.16  | 4773.1217  | [8,8,1,22,1] | 3.09  | 4773.1070  | 2 | 3490949 |
| 0.13  | 5285.6111  | [8,8,1,30,0] | 1.34  | 5285.6182  | 1 | 3357 |
| 0.13  | 5245.1453  | [9,9,1,24,0] | 1.49  | 5245.1375  | 1 | 565 |
|  |  |  |  |  |  |  |  |
| Replicate 3 | 0.13  | 3989.2854  | [8,8,1,14,0] | 0.70  | 3989.2826  | 1 | 3280 |
| 0.16  | 4434.9596  | [8,8,1,20,0] | 2.44  | 4434.9704  | 6 | 578756 |
| 0.17  | 4514.9305  | [8,8,1,21,0] | 0.73  | 4514.9272  | 6 | 3122377 |
| 0.12  | 4573.9685  | [8,8,1,21,1] | 0.92  | 4573.9643  | 2 | 5242 |
| 0.53  | 4765.1635  | [8,8,1,22,0] | 2.93  | 4765.1495  | 8 | 18481026 |
| 0.15  | 4756.0944  | [8,8,1,22,1] | 2.93  | 4756.0804  | 2 | 2660006 |
| 0.12  | 5370.7710  | [8,8,1,30,0] | 3.73  | 5370.7509  | 1 | 2322 |
| 0.12  | 5177.0567  | [9,9,1,24,0] | 4.91  | 5177.0313  | 1 | 1726 |