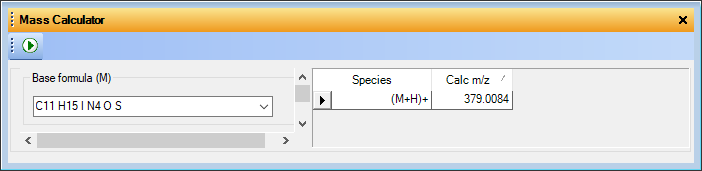
Sample #3, by positive ion ElectrosprayPredicted m/z:



|  |  |  |  |
| --- | --- | --- | --- |
| m/z | Abund | Abund % |  |
| 98.9608 | 502.56 | 1.19 |  |
| 104.0499 | 461.14 | 1.1 |  |
| 105.0581 | 506.23 | 1.2 |  |
| 133.9293 | 332.13 | 0.79 |  |
| 136.972 | 377.56 | 0.9 |  |
| 210.0228 | 1232.61 | 2.93 |  |
| 230.9595 | 607.95 | 1.44 |  |
| 231.9609 | 8216.22 | 19.52 |  |
| 232.0097 | 392.16 | 0.93 |  |
| 232.961 | 581.25 | 1.38 |  |
| 252.9711 | 417.11 | 0.99 |  |
| 308.9747 | 1126.33 | 2.68 |  |
| 316.9872 | 321.87 | 0.76 |  |
| 319.9595 | 1868.09 | 4.44 |  |
| 359.9883 | 739.22 | 1.76 |  |
| 369.4991 | 669.16 | 1.59 |  |
| 376.0174 | 570.07 | 1.35 |  |
| 378.0004 | 1951.8 | 4.64 |  |
| 378.4999 | 655.73 | 1.56 |  |
| 379.0072 | 11890 | 28.25 |  |
| 379.0618 | 776.56 | 1.84 |  |
| 379.0814 | 481.02 | 1.14 |  |
| 380.0095 | 1344.41 | 3.19 |  |
| 381.0048 | 645.37 | 1.53 |  |
| 399.0232 | 42094.81 | 100 |  |
| 399.1079 | 636.9 | 1.51 |  |
| 399.1609 | 563.84 | 1.34 |  |
| 399.524 | 13243.77 | 31.46 |  |
| 399.5884 | 930.87 | 2.21 |  |
| 400.0228 | 5453.15 | 12.95 |  |
| 400.0796 | 382.27 | 0.91 |  |
| 400.5219 | 1465.99 | 3.48 |  |
| 401.0131 | 513.51 | 1.22 |  |
| 419.0402 | 1891.17 | 4.49 |  |
| 420.0383 | 352.51 | 0.84 |  |
| 435.0699 | 11368.52 | 27.01 |  |
| 435.1466 | 312.68 | 0.74 |  |
| 435.3629 | 550.97 | 1.31 |  |
| 435.695 | 409.68 | 0.97 |  |
| 436.0724 | 2093.91 | 4.97 |  |
| 436.1282 | 357.13 | 0.85 |  |
| 437.0638 | 964.48 | 2.29 |  |
| 443.021 | 755.41 | 1.79 |  |
| 443.5217 | 338.11 | 0.8 |  |
| 449.0834 | 1317.17 | 3.13 |  |
| 450.0863 | 375.73 | 0.89 |  |
| 451.0716 | 300.95 | 0.71 |  |
| 457.0531 | 343.87 | 0.82 |  |
| 474.991 | 691.28 | 1.64 |  |
| 506.531 | 448.33 | 1.07 |  |
| 507.041 | 671.55 | 1.6 |  |
| 525.0479 | 4900.66 | 11.64 |  |
| 526.0519 | 954.55 | 2.27 |  |
| 527.0443 | 441.87 | 1.05 |  |
| 547.027 | 462.88 | 1.1 |  |
| 652.0408 | 1108.21 | 2.63 |  |
| 652.5411 | 574.51 | 1.36 |  |
| 653.0308 | 328.94 | 0.78 |  |
| 737.9883 | 405.93 | 0.96 |  |
| 754.9922 | 943.43 | 2.24 |  |
| 755.9933 | 396.33 | 0.94 |  |
| 790.9671 | 669.56 | 1.59 |  |
| 792.9731 | 486.73 | 1.16 |  |
| 797.0394 | 20089.49 | 47.72 |  |
| 798.0411 | 6182.87 | 14.69 |  |
| 799.0382 | 2714.91 | 6.45 |  |
| 800.0381 | 663.98 | 1.58 |  |
| 819.021 | 417.34 | 0.99 |  |
| 833.0163 | 12646.47 | 30.04 |  |
| 833.1222 | 534.37 | 1.27 |  |
| 834.0176 | 3988.57 | 9.48 |  |
| 835.0127 | 5465.35 | 12.98 |  |
| 835.1321 | 337.66 | 0.8 |  |
| 836.0144 | 1642.78 | 3.9 |  |
| 837.0108 | 635.05 | 1.51 |  |
| 849.0473 | 436.91 | 1.04 |  |
| 855.0012 | 796.22 | 1.89 |  |
| 855.9962 | 321.58 | 0.76 |  |
| 856.992 | 436.3 | 1.04 |  |
| 885.0381 | 770.62 | 1.83 |  |
| 890.9644 | 522.35 | 1.24 |  |
| 892.9682 | 404.93 | 0.96 |  |
| 897.089 | 529.44 | 1.26 |  |
| 906.9518 | 322.82 | 0.77 |  |
| 911.0334 | 696.51 | 1.65 |  |
| 912.0389 | 333.29 | 0.79 |  |
| 922.1097 | 793.24 | 1.88 |  |
| 942.918 | 408.65 | 0.97 |  |
| 944.9043 | 417.08 | 0.99 |  |
| 984.9514 | 320.86 | 0.76 |  |
| 1246.9927 | 361.8 | 0.86 |  |
| 1303.0423 | 311.94 | 0.74 |  |
| 1339.0375 | 588.22 | 1.4 |  |
| 1340.0337 | 348.89 | 0.83 |  |
| 1341.045 | 445.46 | 1.06 |  |
| 1357.045 | 378.96 | 0.9 |  |
| 1700.9981 | 335.09 | 0.8 |  |
| 1702.9974 | 639.18 | 1.52 |  |
| 1703.9965 | 308.52 | 0.73 |  |
| 1704.9942 | 360.31 | 0.86 |  |