Aqueous Alkaline Phosphate Facilitates the Non-exchangeable Deuteration of Peptides and Proteins

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Part I. Data Analysis.

Peptide:

The average mass of peptide is calculated by taking the average mass of all the isotopic peaks weighted by their intensities. This means that for an isotopic peak distribution containing n peaks the average mass (M) can be found using Equation 1

Equation 1:

$$\mathrm{M}_{deuterium} = \frac{\sum_{i=1}^{n} \mathrm{I_i} \cdot M_i}{\sum_{i=1}^{n} \mathrm{I_i}}$$

$$\mathrm{M}_{un-deuterium} = \frac{\sum_{i=1}^{n} \mathrm{I_i} \cdot M_i}{\sum_{i=1}^{n} \mathrm{I_i}}$$

$$\frac{\mathrm{Deuterium}}{molecular} = (\mathrm{M}_{deuterium} - \mathrm{M}_{un-deuterium}) * charge$$

Protein:

$$\mathrm{Deuterium\ mass} = [({}^{m}/_{Z})_{deuterium} - ({}^{m}/_{Z})_{undeuterium}] * z$$

where $({}^{m}/_{Z})_{deuterium}$ is the centroid mass of the fragment ions of interest, whereas $({}^{m}/_{Z})_{undeuterium}$ is the corresponding reference data for completely unlabeled samples fragment ions.

All biochemical graphs were produced using OriginPro 2019b (OriginLab) or R script.

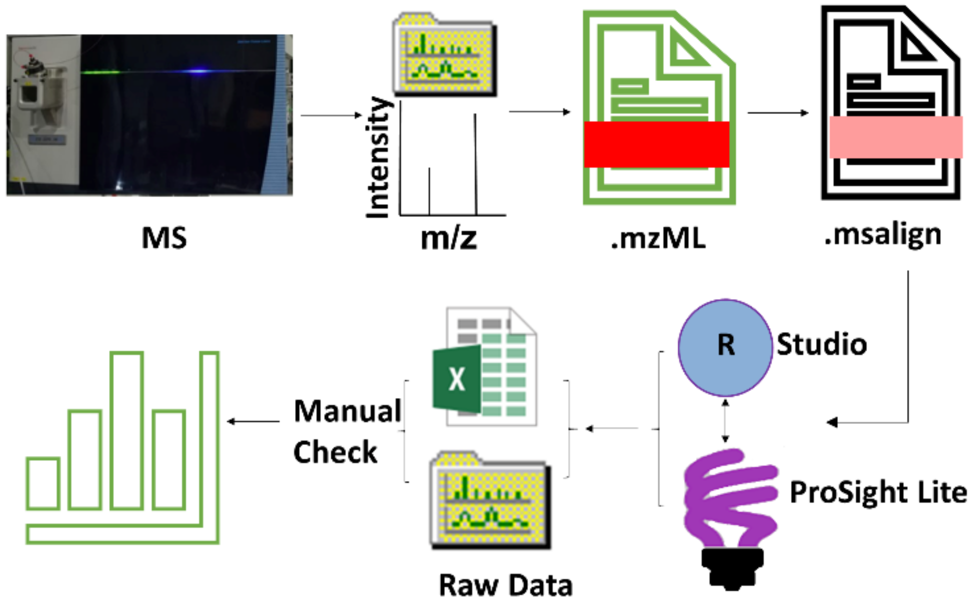
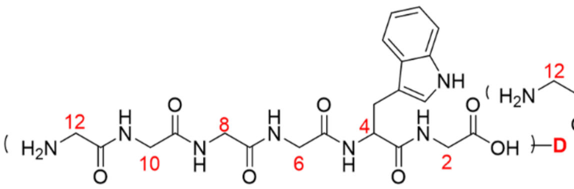


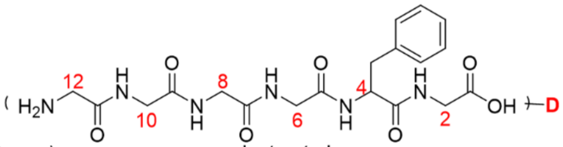
Figure S 1 Data analysis flowchart

These Mb regions include: N-terminus (Gly 1 to Ser 3), A-helix (Asp 4 to Ala 19), B-helix (Asp 20 to Gly 35), C-helix (His 36 to Lys 42), CD loop (Phe 43 to Lys 50), D-helix (Thr 51 to Ala 57), E-helix (Ser 58 to Lys 77), EF loop (Lys 78 to Glu 85), F-helix (Leu 86 to Ala 94), FG loop (Thr 95 to Ile 99), G-helix (Pro 100 to Lys 118), GH loop (His 119 to Phe 123), H-helix (Gly 124 to Gly 150), and C terminus (Phe 151 to Gly 153).

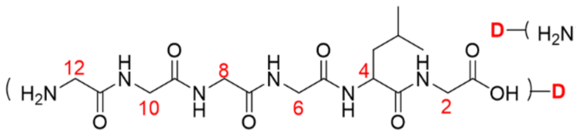
Part II. Supplementary Figures



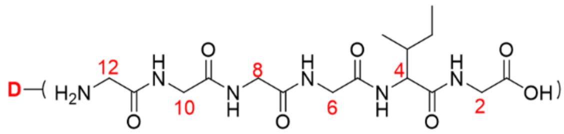
un-deuterated
Chemical Formula: $C_{21}H_{27}N_7O_7$
Exact Mass: 489.1972
Gly-Gly-Gly-Gly-Trp-Gly
(RT 8h, 1.8 Deuterium Incorporation)



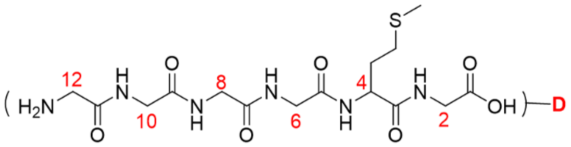
un-deuterated
Chemical Formula: $C_{19}H_{26}N_6O_7$
Exact Mass: 450.1863
Gly-Gly-Gly-Gly-Phe-Gly
(RT 8h, 1.54 Deuterium Incorporation)



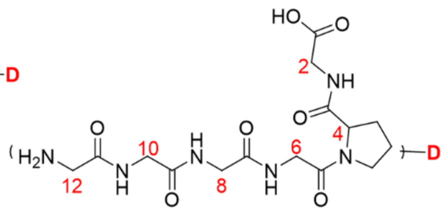
un-deuterated
Chemical Formula: $C_{16}H_{28}N_6O_7$
Exact Mass: 416.2019
Gly-Gly-Gly-Gly-Leu-Gly
(RT 8h, 1.57 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{16}H_{28}N_6O_7$
Exact Mass: 416.2019
Gly-Gly-Gly-Gly-Ile-Gly
(RT 8h, 1.49 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{15}H_{26}N_6O_7S$
Exact Mass: 434.1584
Gly-Gly-Gly-Gly-Met-Gly
(RT 8h, 1.84 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{15}H_{24}N_6O_7$
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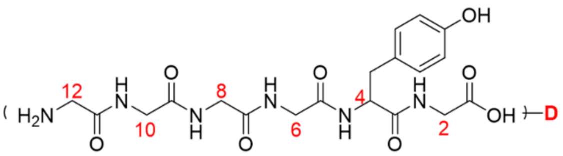
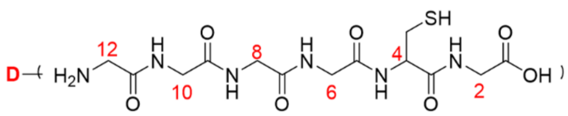
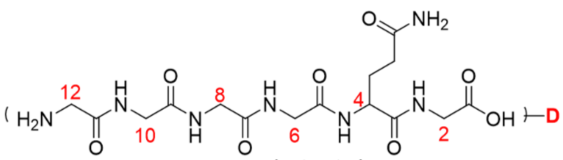
Gly-Gly-Gly-Gly-Pro-Gly
(RT 8h, 2.4 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{19}H_{26}N_6O_8$
Exact Mass: 466.1812
Gly-Gly-Gly-Gly-Tyr-Gly
(RT 8h, 1.61 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{13}H_{22}N_6O_7S$
Exact Mass: 406.1271
Gly-Gly-Gly-Gly-Cys-Gly
(RT 8h, 1.1 Deuterium Incorporation)



un-deuterated
Chemical Formula: $C_{15}H_{25}N_7O_8$
Exact Mass: 431.1765
Gly-Gly-Gly-Gly-Gln-Gly
(RT 8h, 1.84 Deuterium Incorporation)

Figure S2 Hexa-peptides deuteration (backbone deuteration)

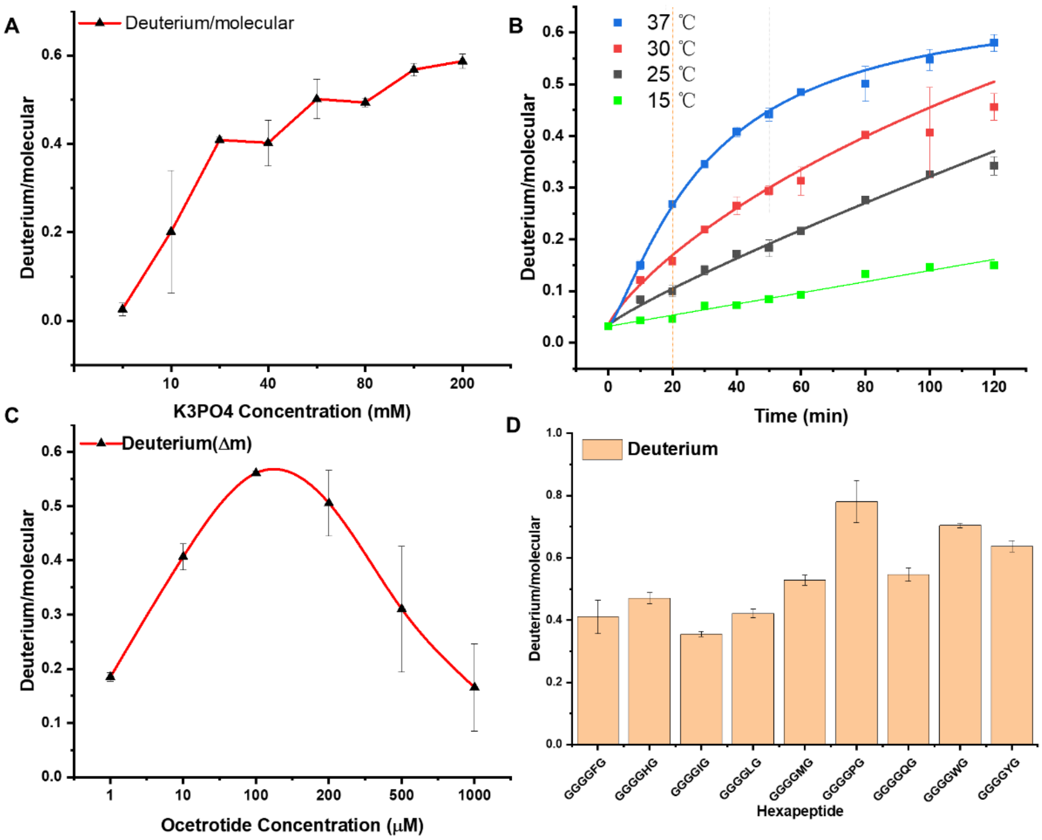


Figure S3 The investigation of optimal conditions for the deuteration of octreotide, including: A) potassium phosphate concentration, B) reaction time at 50 mM potassium phosphate condition, C) octreotide concentration (50 mM potassium phosphate), and D) the deuteration rates of standard hexapeptides at 2 hours. (Triple parallel experiments)

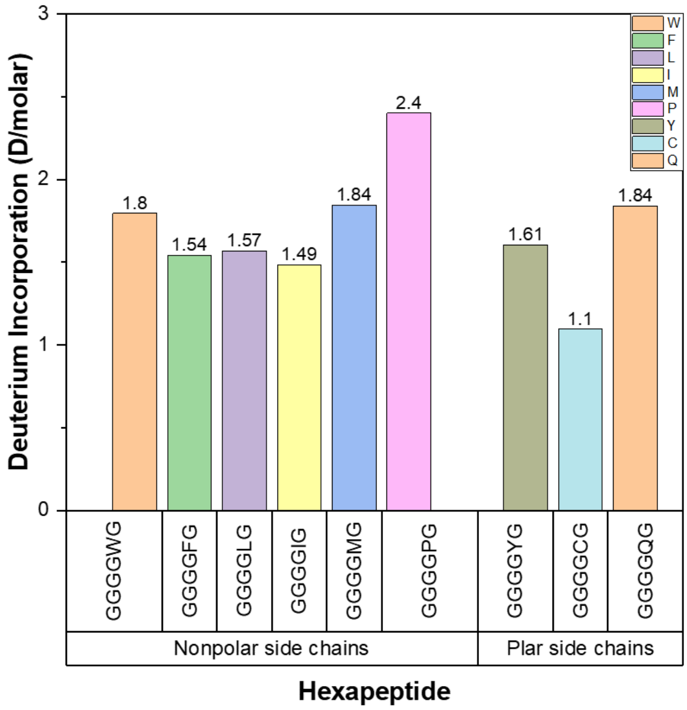
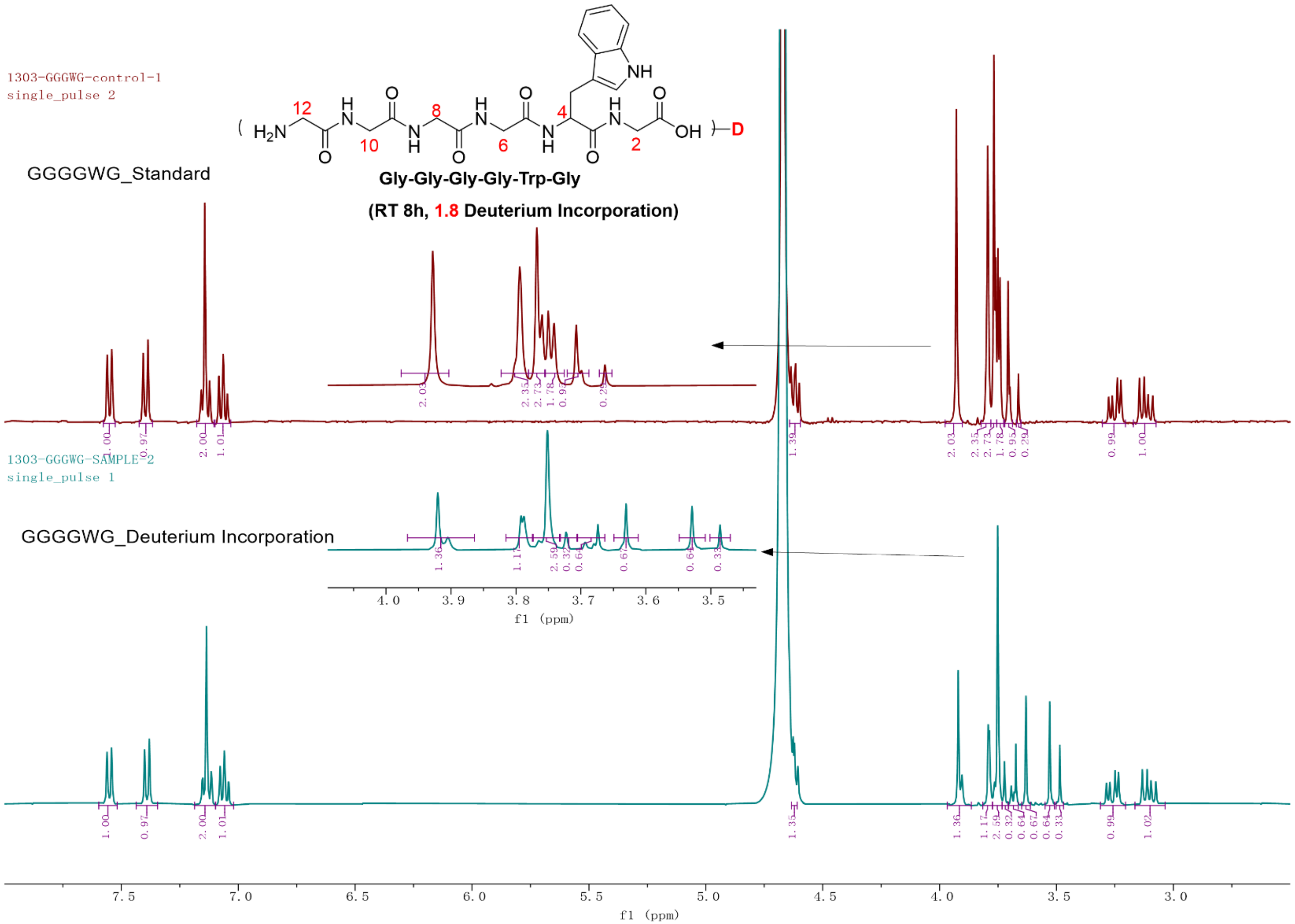
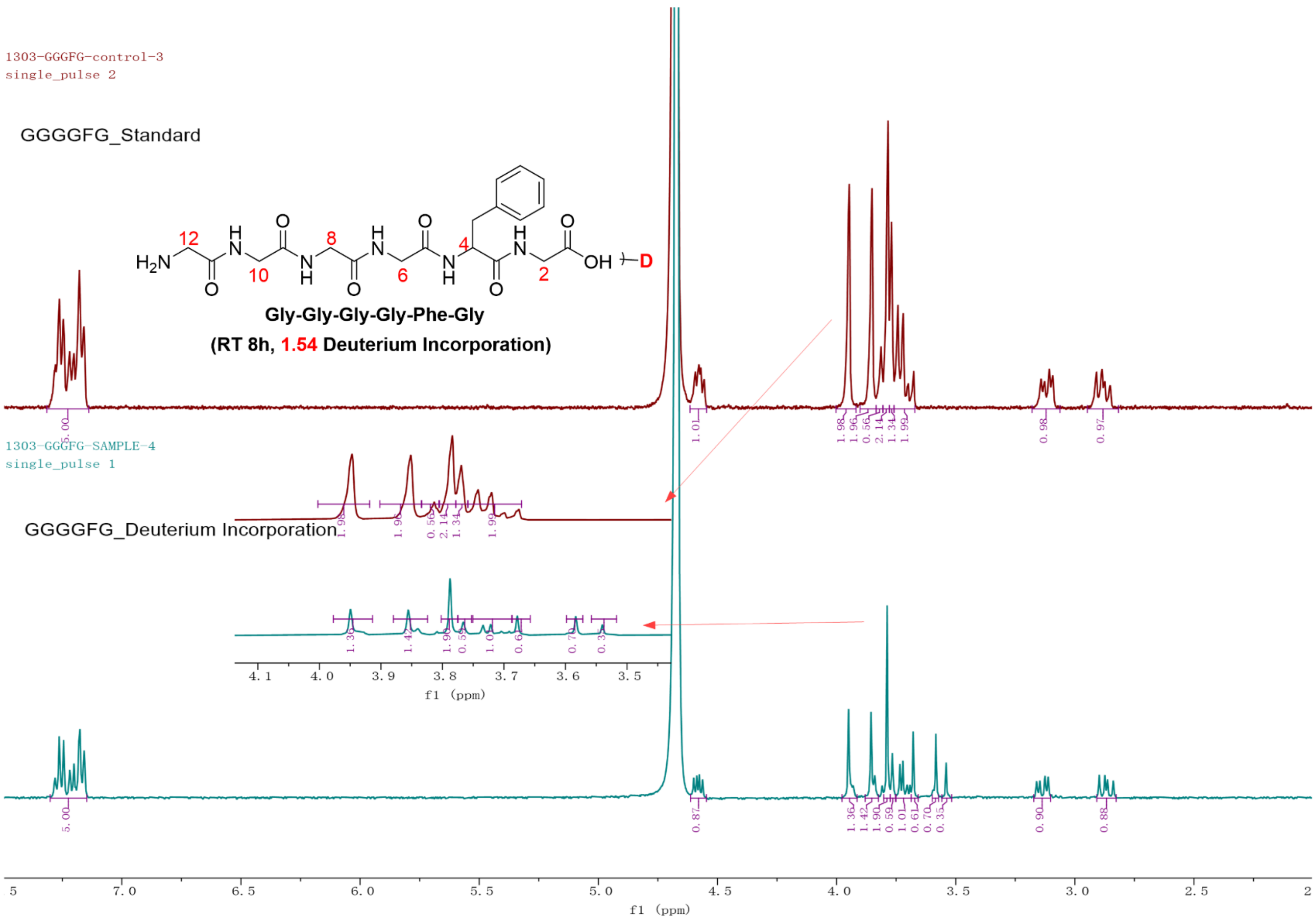


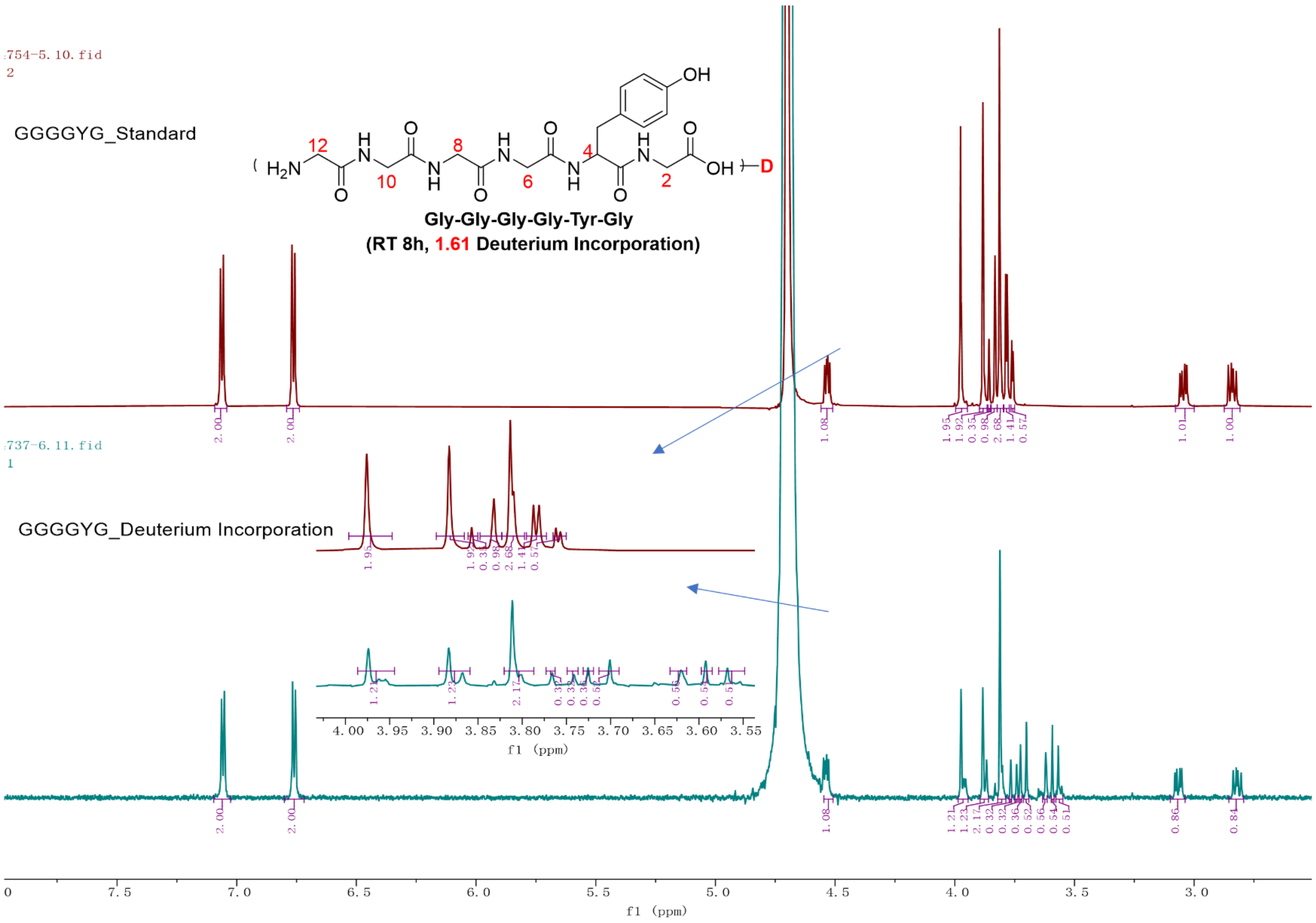
Figure S4 The deuterium incorporation of hexapeptide at 8 h (100 mM potassium phosphate).

Part III. Supporting Information NMR Part

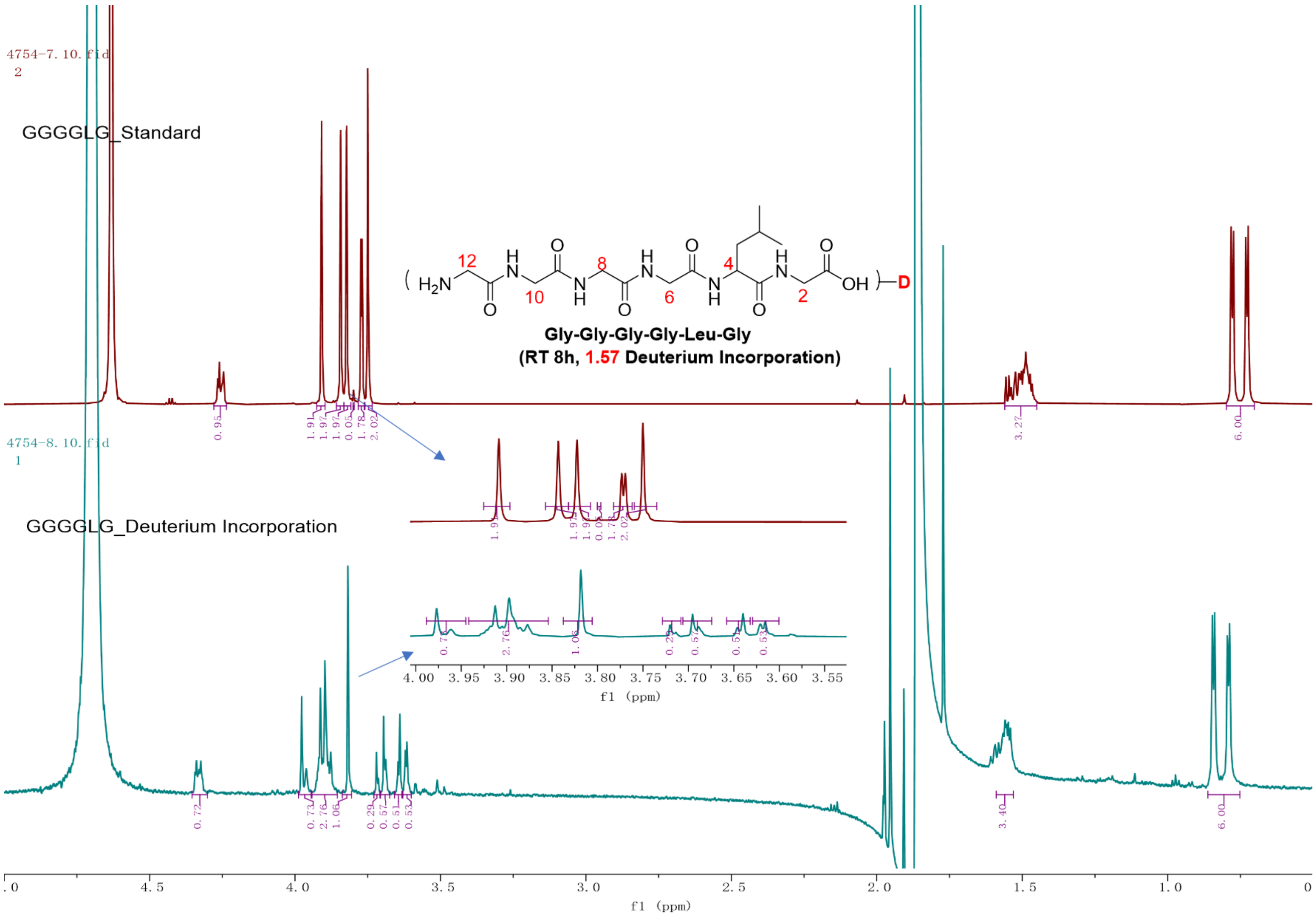
Figure S5 ^{1}HNMR stacked spectra demonstrating the selective backbone deuteration of standard hexapeptides.

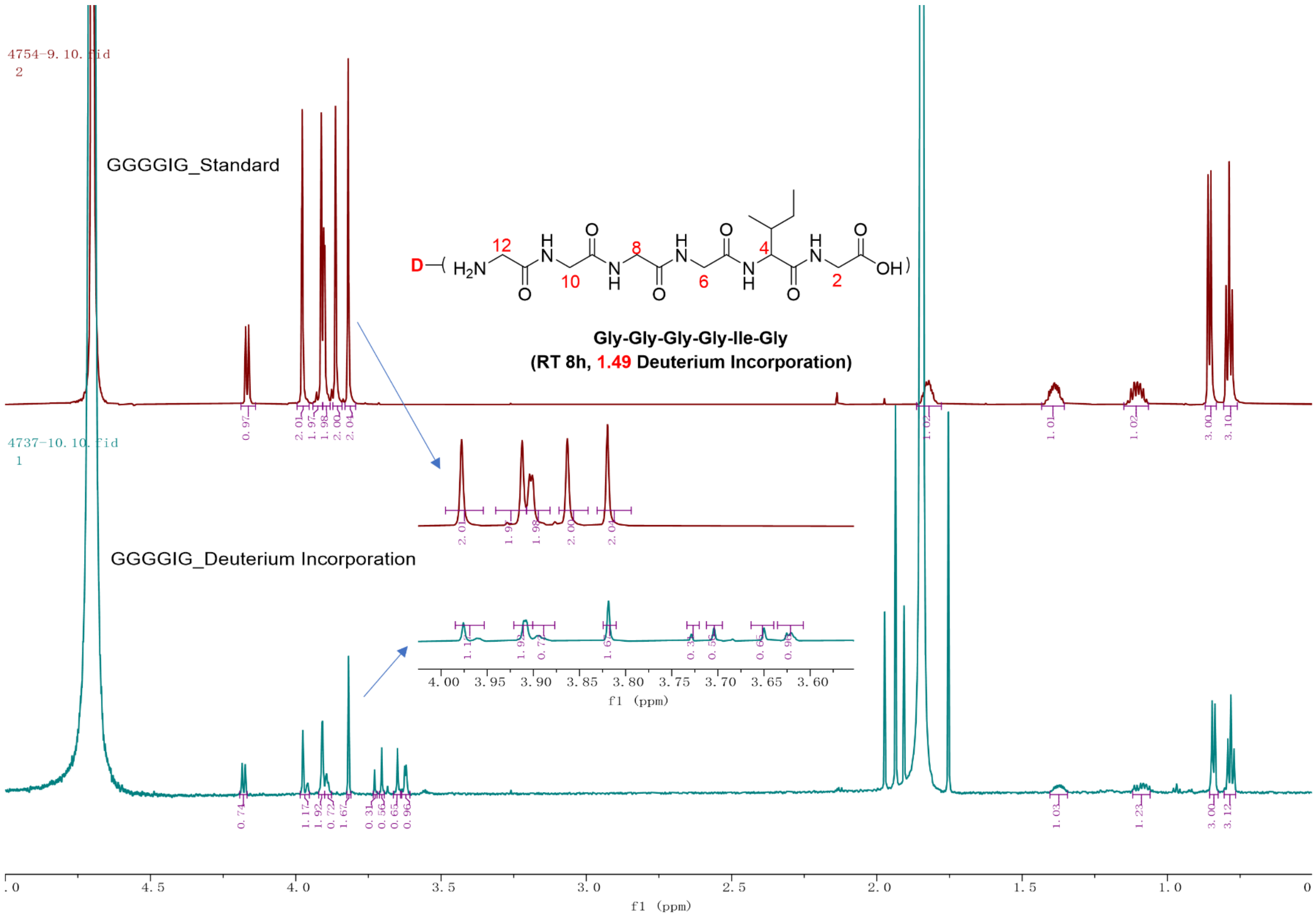

1303-GGGWG-control-1
single_pulse 2
GGGGWG_Standard
Gly-Gly-Gly-Gly-Trp-Gly
(RT 8h, 1.8 Deuterium Incorporation)
1303-GGGWG-SAMPLE-2
single_pulse 1
GGGGWG_Deuterium Incorporation
f1 (ppm)

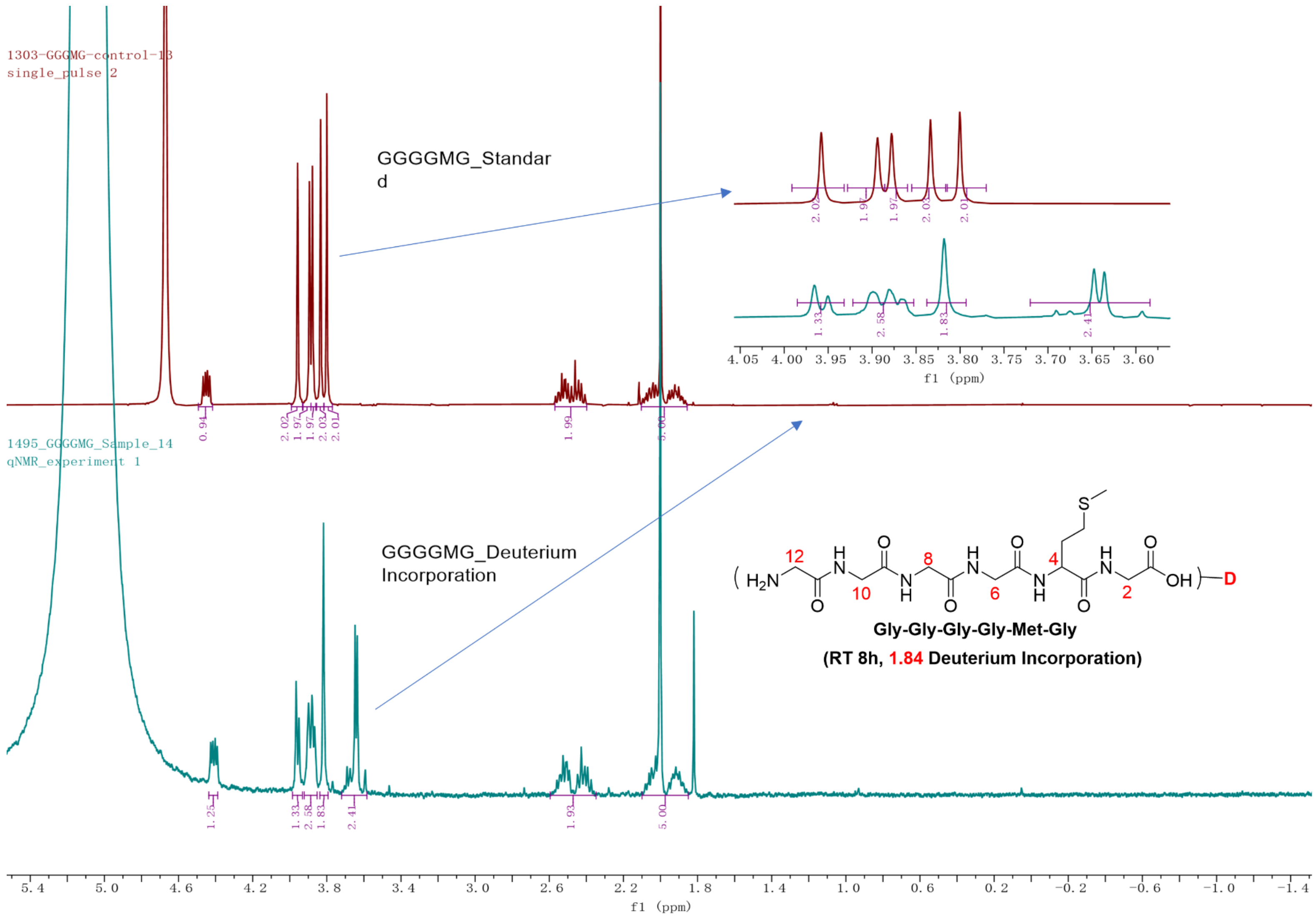

1303-GGGFG-control-3
single_pulse 2
GGGGFG_Standard
Gly-Gly-Gly-Gly-Phe-Gly
(RT 8h, 1.54 Deuterium Incorporation)
1303-GGGFG-SAMPLE-4
single_pulse 1
GGGGFG_Deuterium Incorporation
f1 (ppm)



GGGGYG_Standard
GGGGYG_Deuterium Incorporation
Gly-Gly-Gly-Gly-Tyr-Gly
(RT 8h, 1.61 Deuterium Incorporation)
f1 (ppm)


4754-7.10.fid
2
GGGGLG_Standard
4754-8.10.fid
1
GGGGLG_Deuterium Incorporation
Gly-Gly-Gly-Gly-Leu-Gly
(RT 8h, 1.57 Deuterium Incorporation)
f1 (ppm)


4754-9.10.fid
2
GGGGIG_Standard
4737-10.10.fid
1
GGGGIG_Deuterium Incorporation
D
H2N
OH
12
10
8
6
4
2
Gly-Gly-Gly-Gly-Ile-Gly
(RT 8h, 1.49 Deuterium Incorporation)
f1 (ppm)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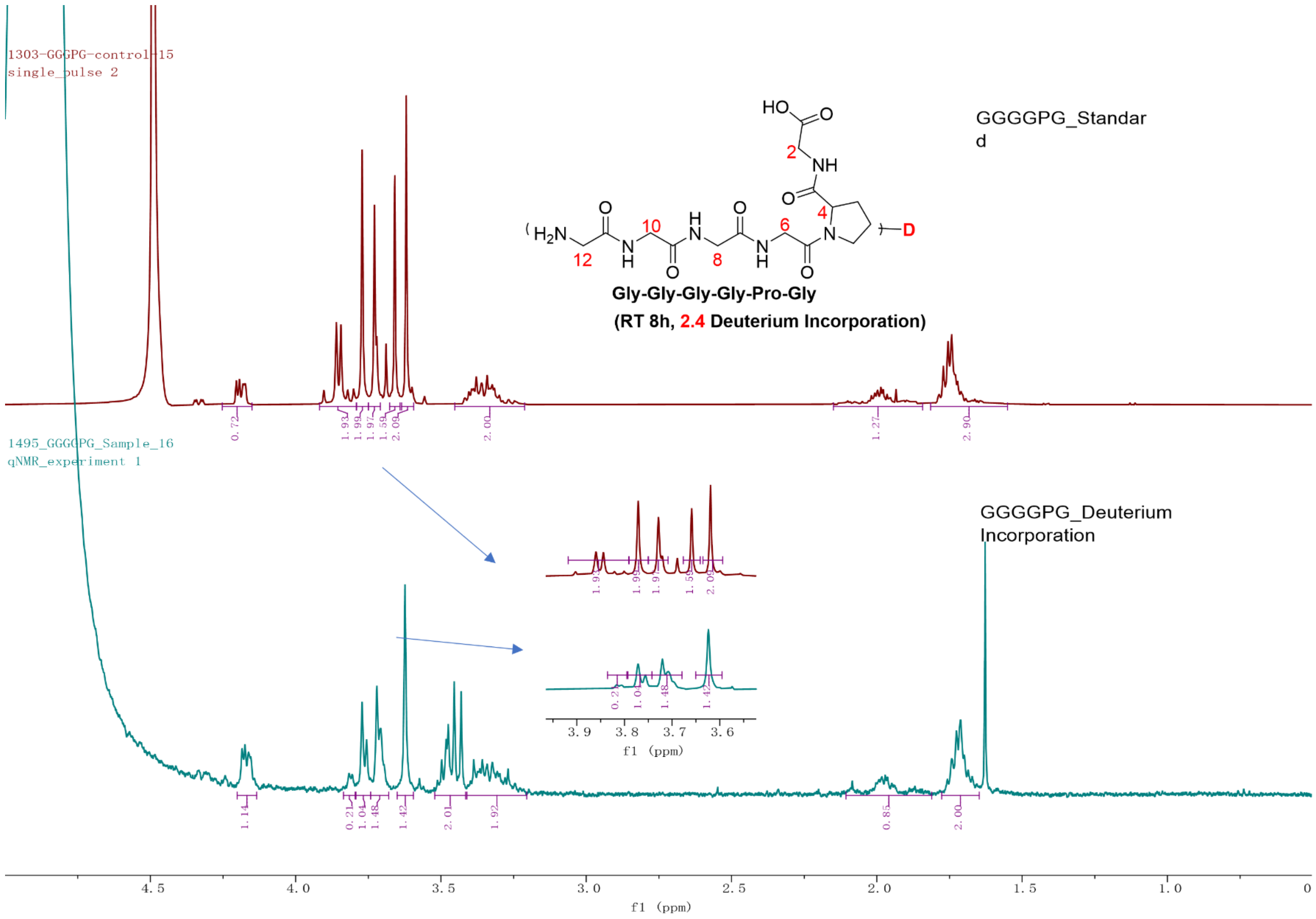
single_pulse 2
GGGGMG_Standard
1495_GGGMG_Sample_14
qNMR_experiment 1
GGGGMG_Deuterium Incorporation
Gly-Gly-Gly-Gly-Met-Gly
(RT 8h, 1.84 Deuterium Incorporation)
f1 (ppm)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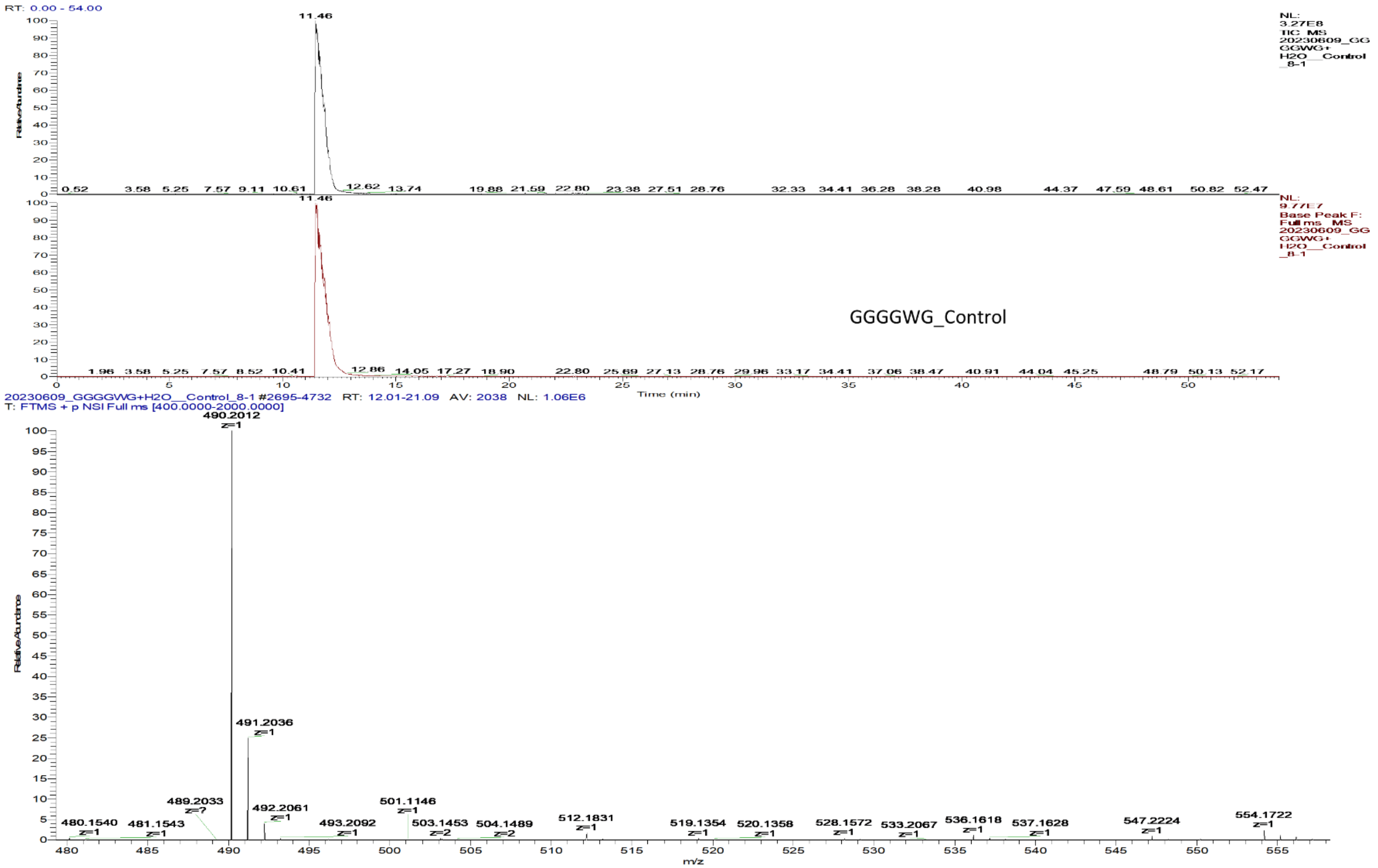
single_pulse 2
GGGGPG_Standar
d
Gly-Gly-Gly-Gly-Pro-Gly
(RT 8h, 2.4 Deuterium Incorporation)
1495_GGGGPG_Sample_16
qNMR_experiment 1
GGGGPG_Deuterium
Incorporation
f1 (ppm)

Part IIII. Supporting Information HPLC-MS/MS Part

Figure S6 The HPLC-MS spectra of the standard hexapeptides.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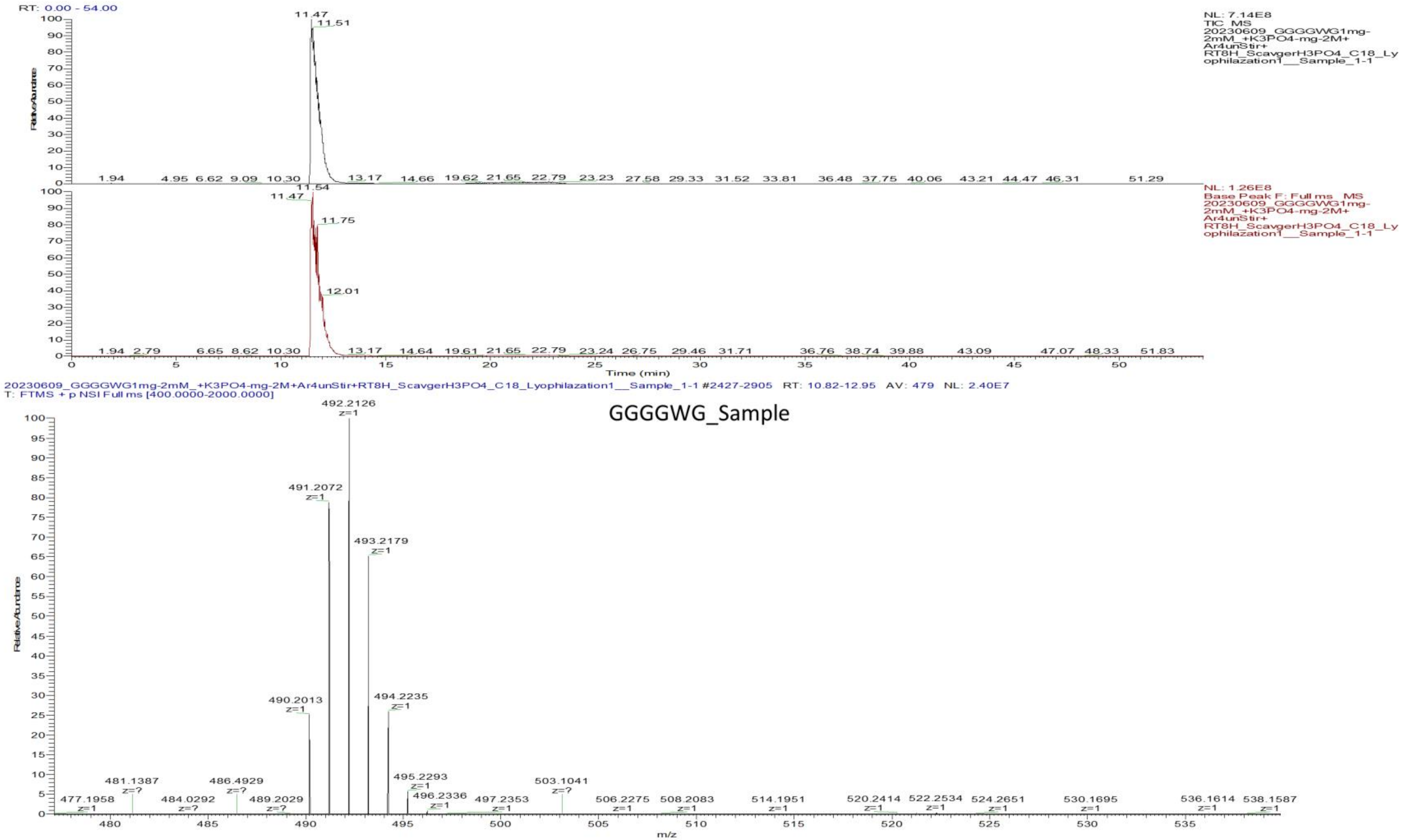
NL: 3.27E8 TIC MS 20230609_GGGGWG+H2O__Control_8-1
NL: 9.77E7 Base Peak F: Full ms MS 20230609_GGGGWG+H2O__Control_8-1
GGGGWG_Control
Time (min)
20230609_GGGGWG+H2O__Control_8-1 #2695-4732 RT: 12.01-21.09 AV: 2038 NL: 1.06E6
T: FTMS + p NSI Full ms [400.0000-2000.0000]
490.2012
491.2036
489.2033
492.2061
501.1146
554.1722
m/z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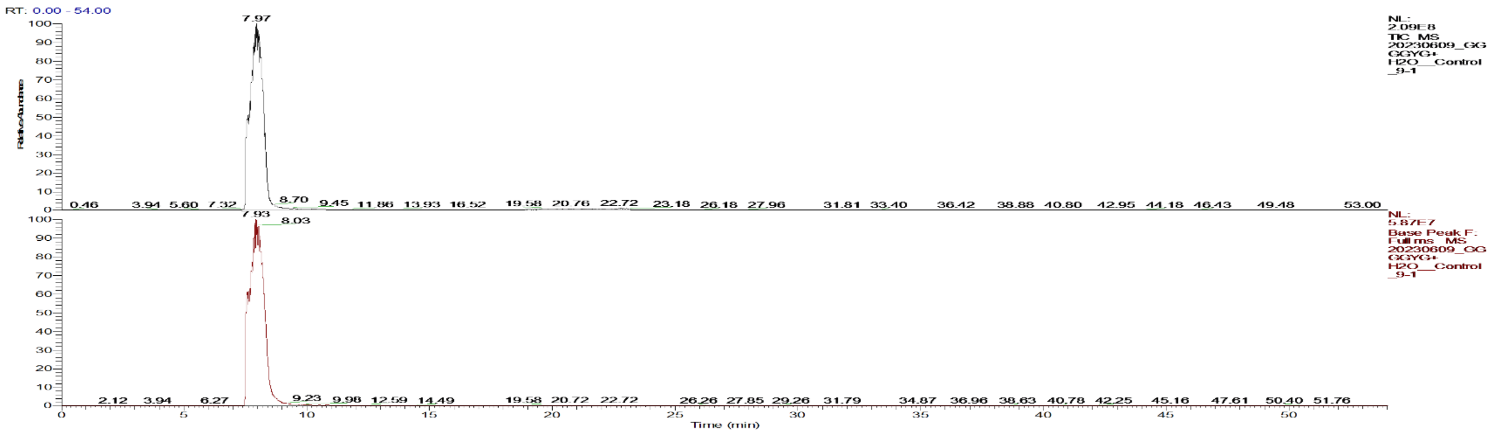
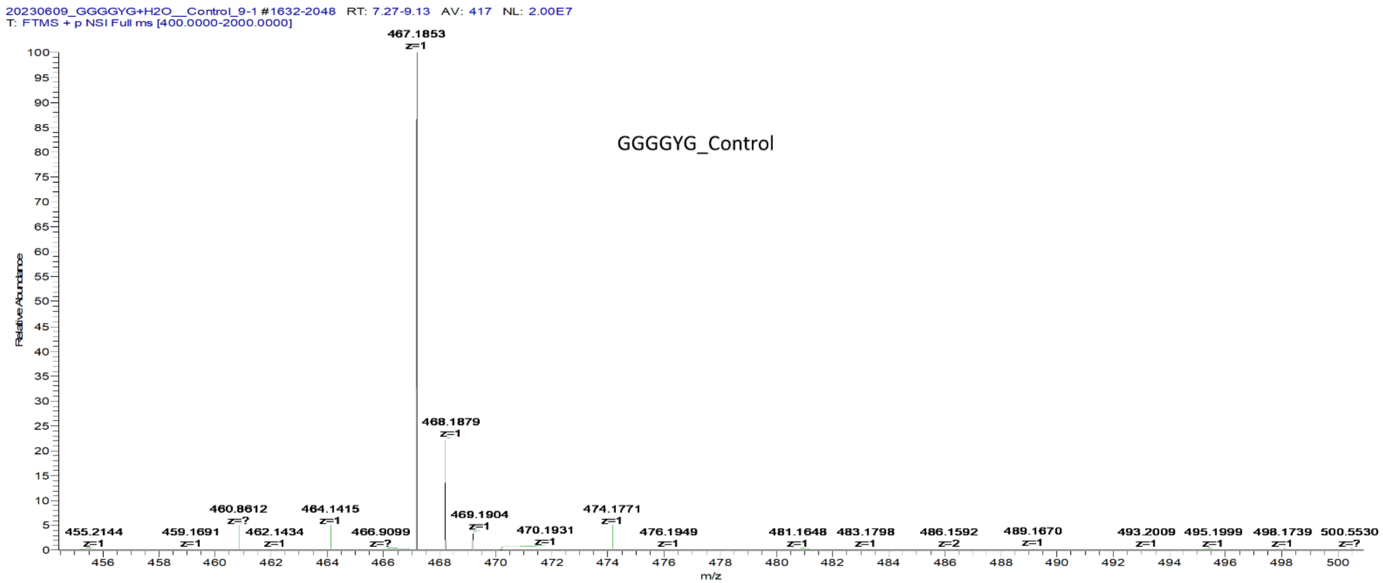
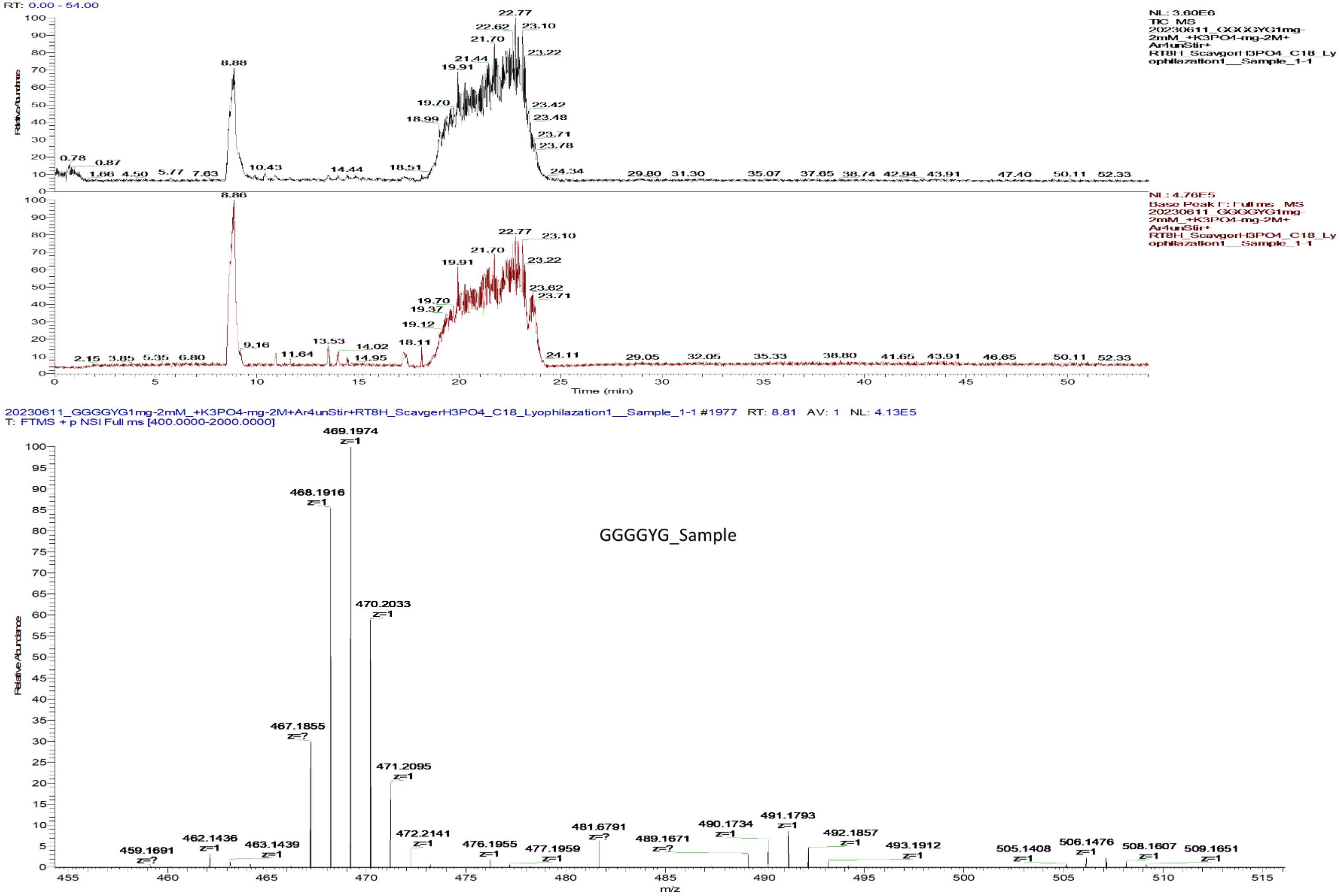
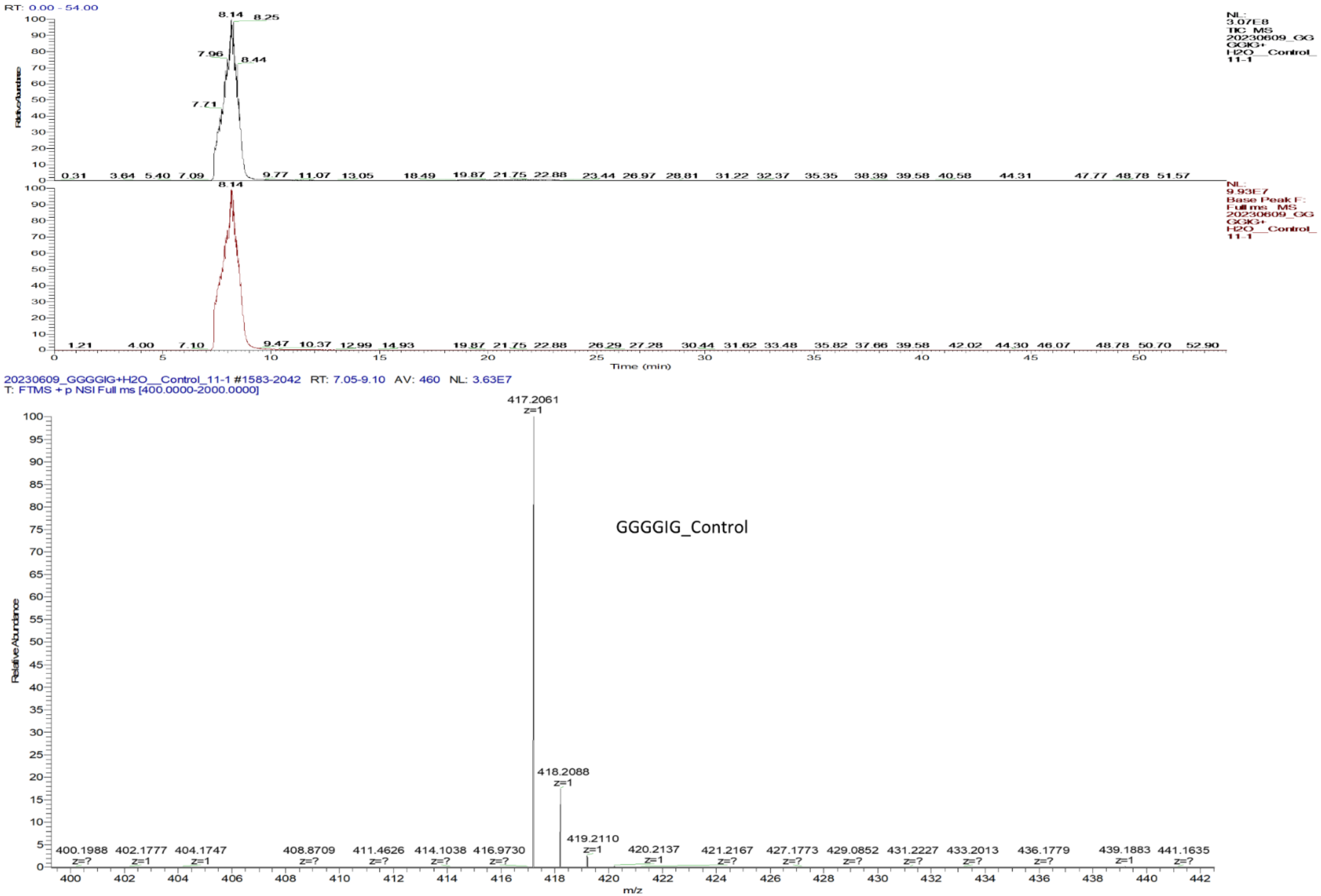
NL: 7.14E8
TIC MS
20230609_GGGGWG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1
NL: 1.26E8
Base Peak F: Full ms MS
20230609_GGGGWG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1
Time (min)
20230609_GGGGWG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1 #2427-2905 RT: 10.82-12.95 AV: 479 NL: 2.40E7
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGWG_Sample
Relative Abundance
m/z
492.2126
491.2072
493.2179
490.2013
494.2235
495.2293
503.1041




GGGGYG_Control


GGGGYG_Sample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NL: 3.07E8 TIC MS 20230609_GGGGIG+H2O__Control_11-1
NL: 9.93E7 Base Peak F: Full ms MS 20230609_GGGGIG+H2O__Control_11-1
Relative Abundance
Time (min)
20230609_GGGGIG+H2O__Control_11-1 #1583-2042 RT: 7.05-9.10 AV: 460 NL: 3.63E7
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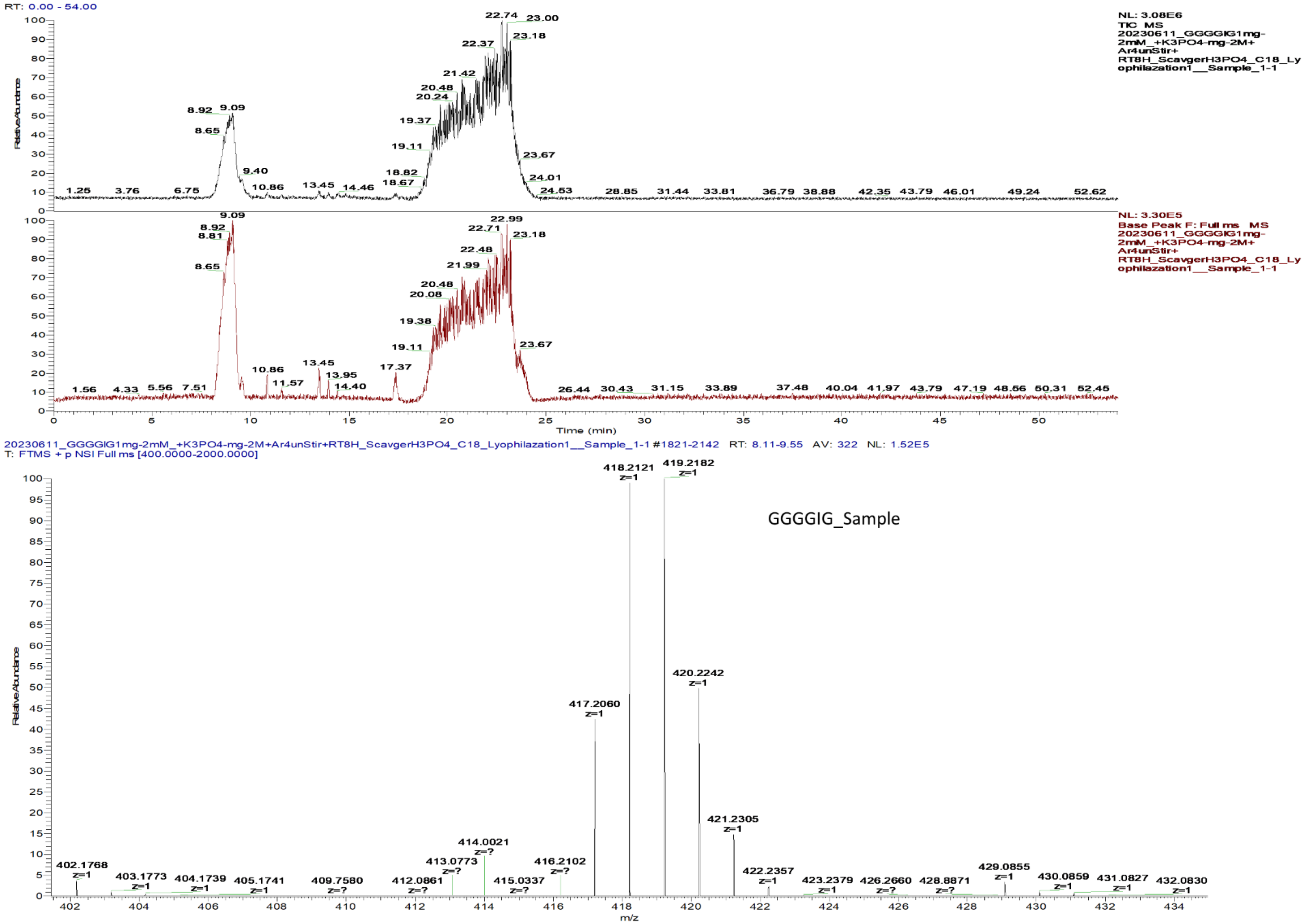
419.2110 z=1
GGGGIG_Control
m/z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TIC MS
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NL: 3.30E5
Base Peak F: Full ms MS
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Relative Abundance
Time (min)
20230611_GGGGIG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1 #1821-2142 RT: 8.11-9.55 AV: 322 NL: 1.52E5
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGIG_Sample
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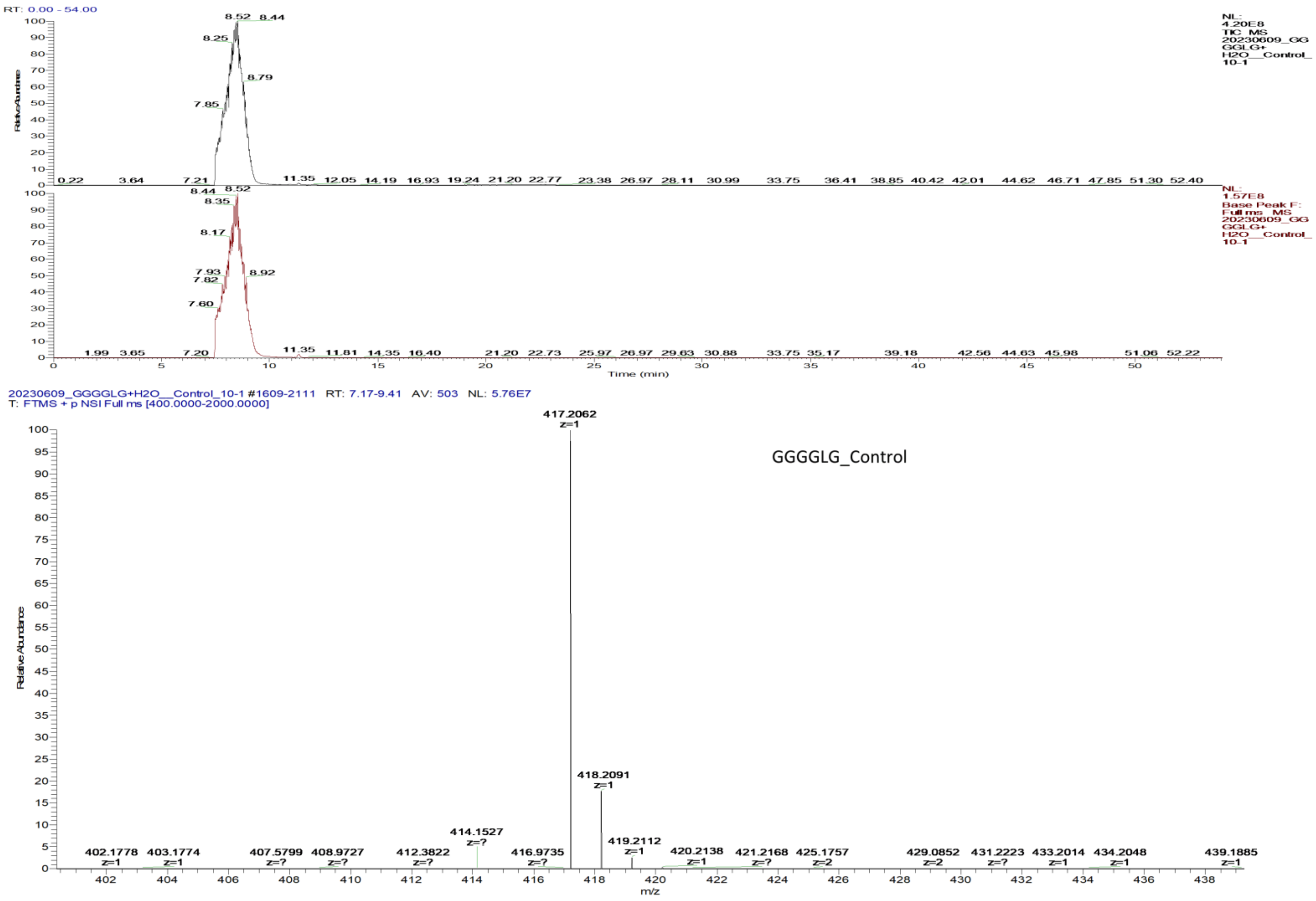
419.2182 z=1
420.2242 z=1
417.2060 z=1
421.2305 z=1
414.0021 z=?
m/z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Time (min)
Relative Abundance
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T: FTMS + p NSI Full ms [400.0000-2000.0000]
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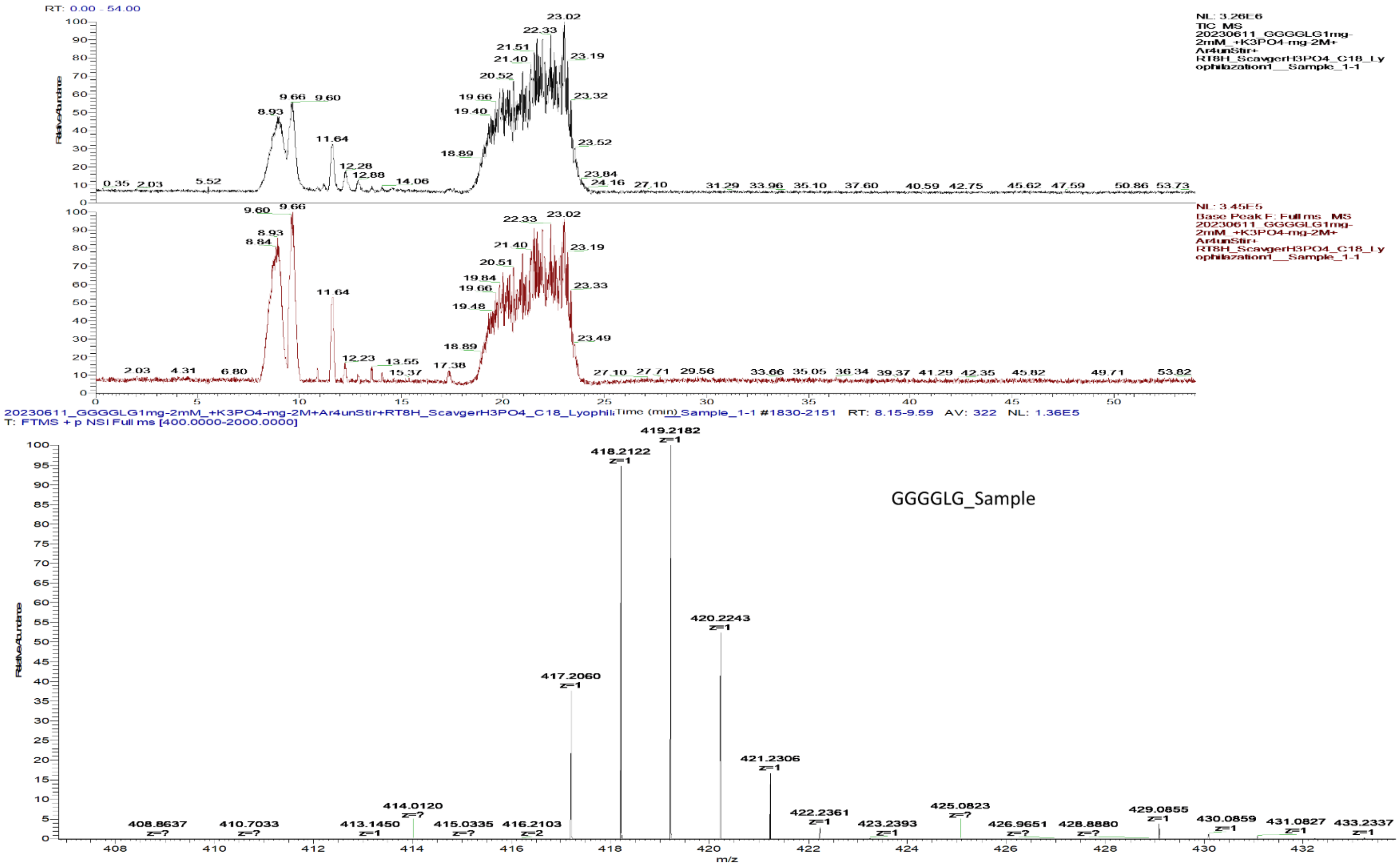
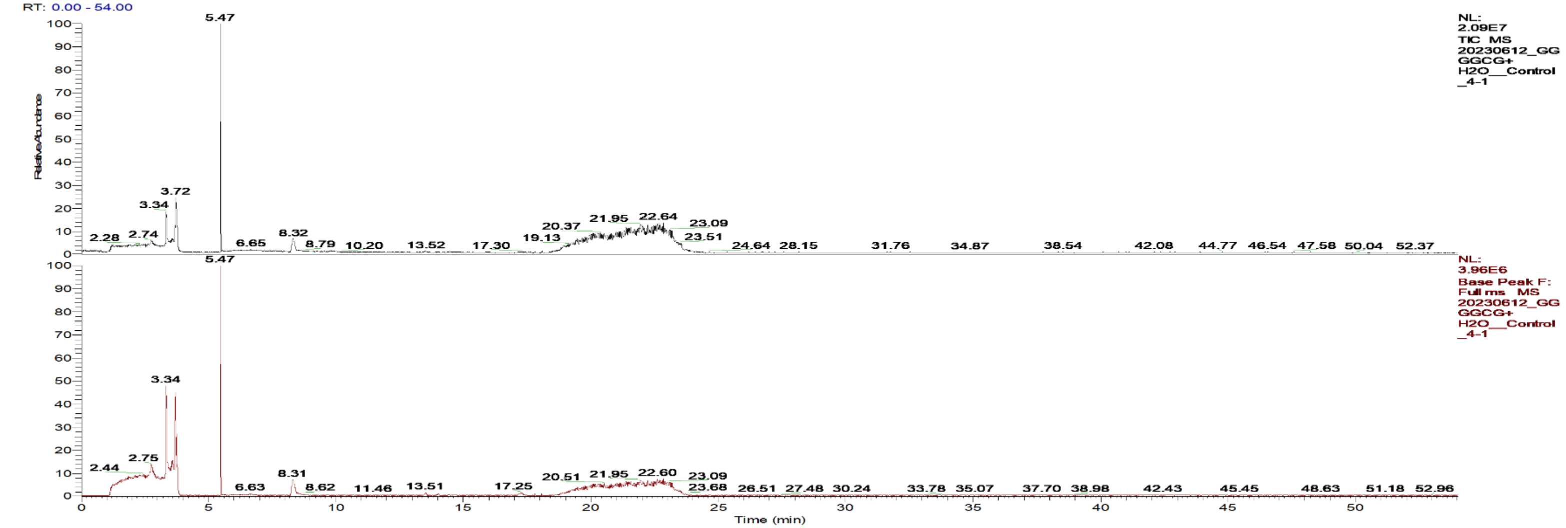
419.2112 z=1
414.1527 z=?
GGGGLG_Control
m/z



GGGGLG_Sample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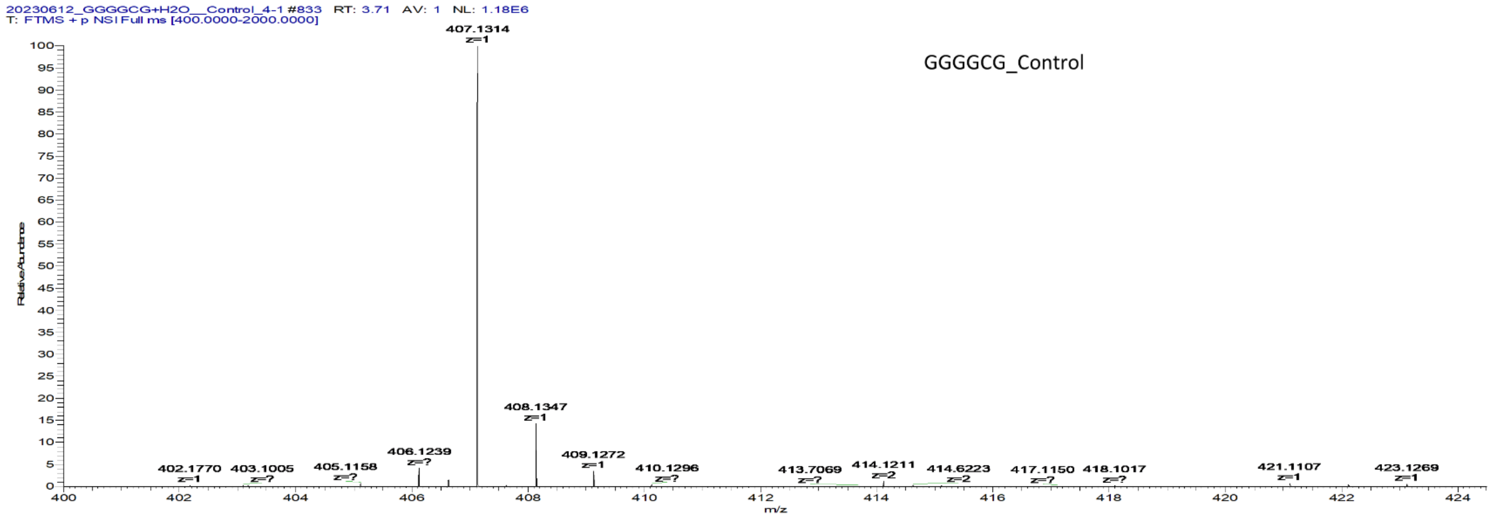
Relative Abundance
Time (min)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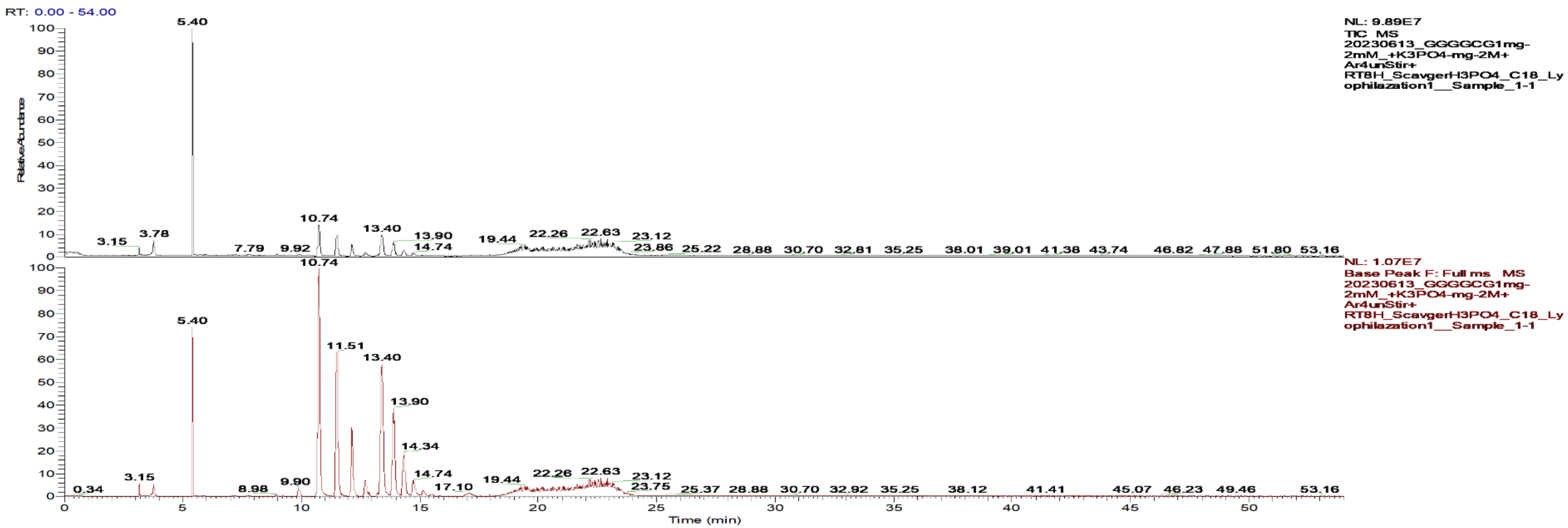
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGCG_Control
407.1314 z=1
408.1347 z=1
406.1239 z=?
409.1272 z=1
Relative Abundance
m/z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NL: 1.07E7
Base Peak F: Full ms MS
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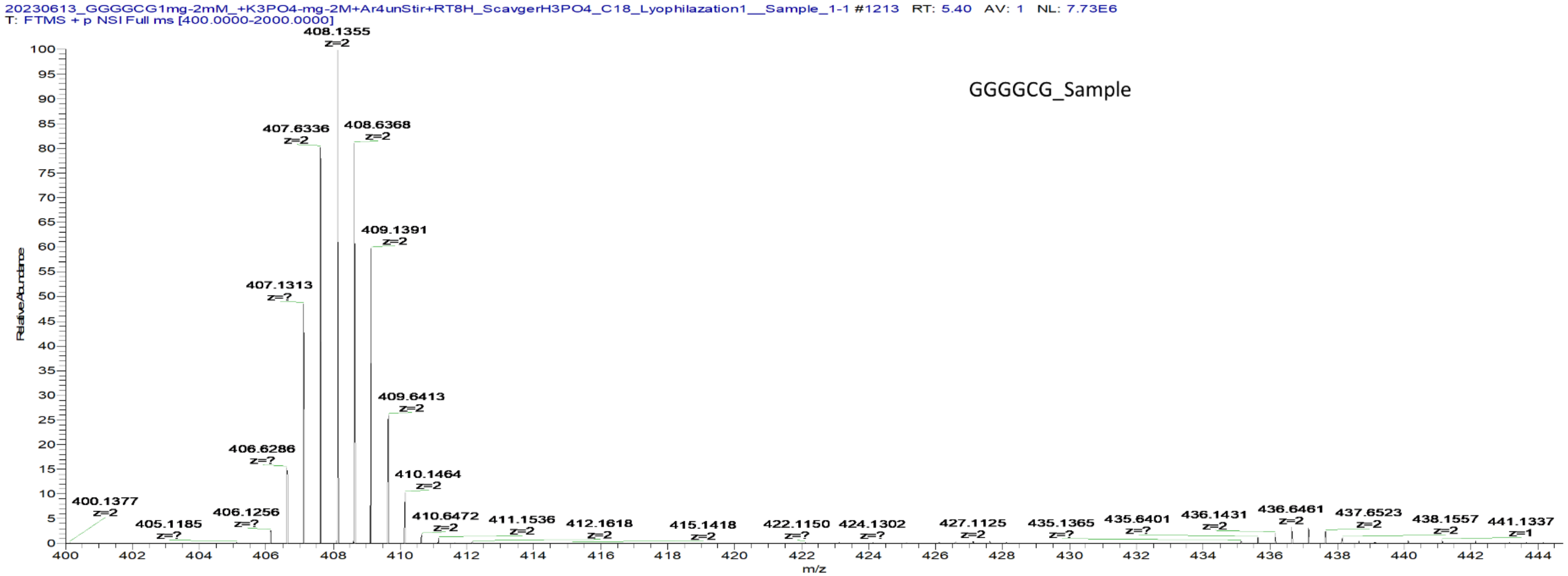
Relative Abundance
Time (min)
5.40
3.15
3.78
7.79
9.92
10.74
13.40
13.90
14.74
19.44
22.26
22.63
23.12
23.86
25.22
28.88
30.70
32.81
35.25
38.01
39.01
41.38
43.74
46.82
47.88
51.80
53.16
0.34
8.98
9.90
11.51
14.34
17.10
23.75
25.37
32.92
38.12
41.41
45.07
46.23
49.46


20230613_GGGGCG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1 #1213 RT: 5.40 AV: 1 NL: 7.73E6
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGCG_Sample
Relative Abundance
m/z
408.1355 z=2
407.6336 z=2
408.6368 z=2
409.1391 z=2
407.1313 z=?
409.6413 z=2
406.6286 z=?
410.1464 z=2
400.1377 z=2
405.1185 z=?
406.1256 z=?
410.6472 z=2
411.1536 z=2
412.1618 z=2
415.1418 z=2
422.1150 z=?
424.1302 z=?
427.1125 z=2
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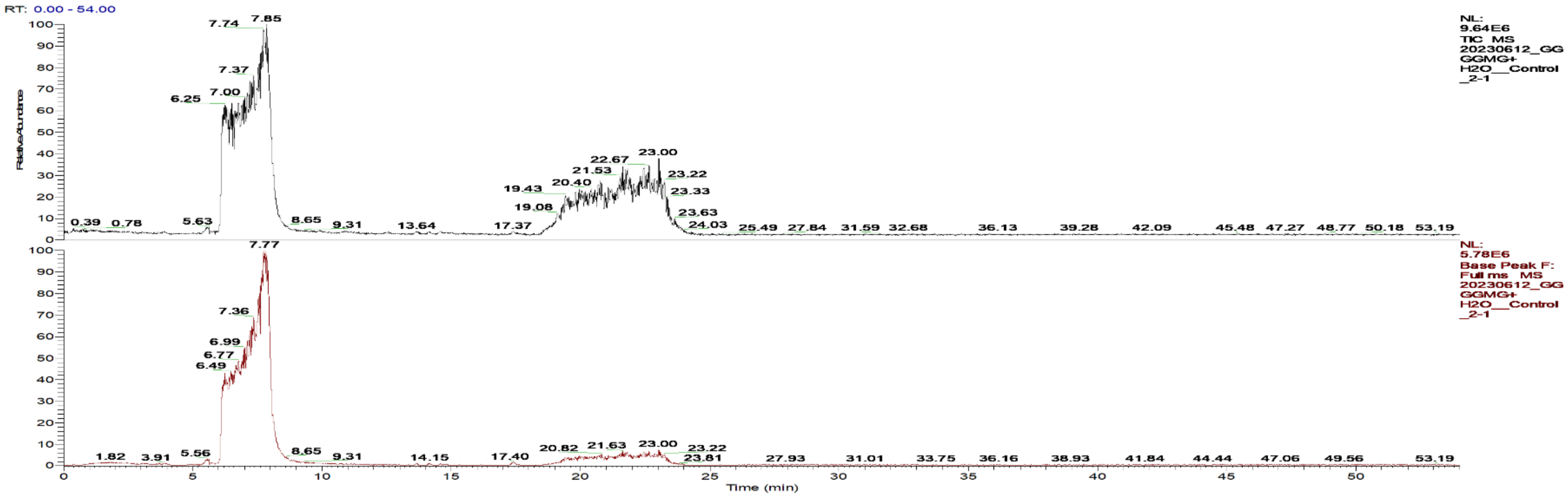
441.1337 z=1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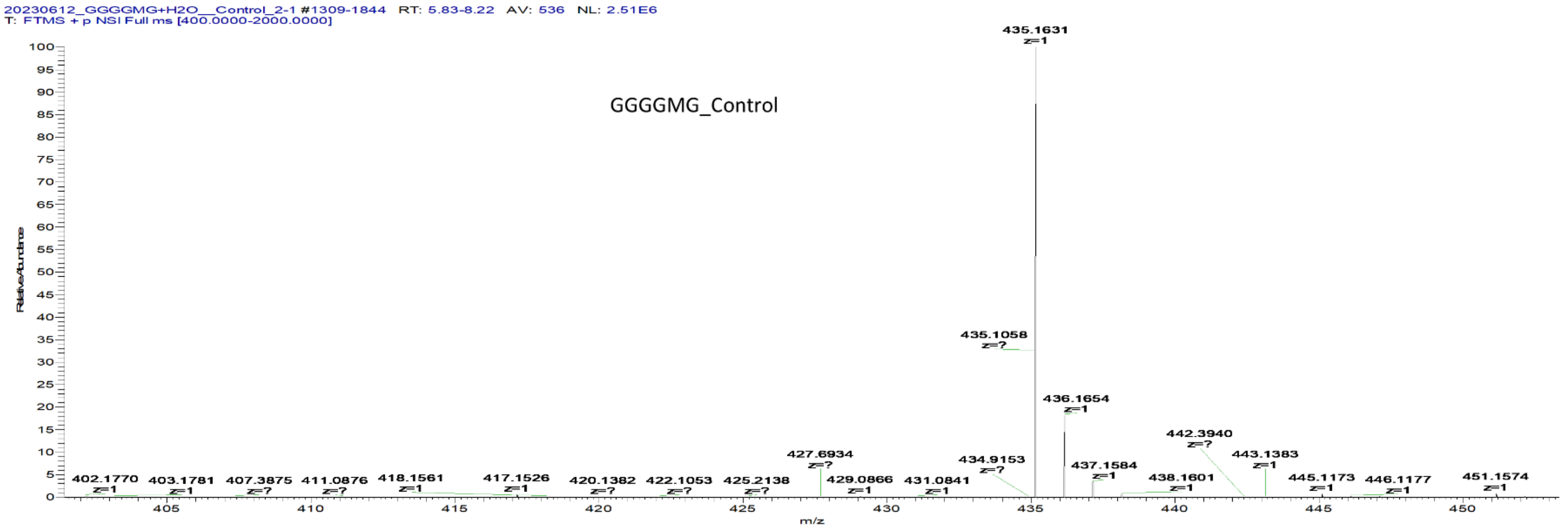
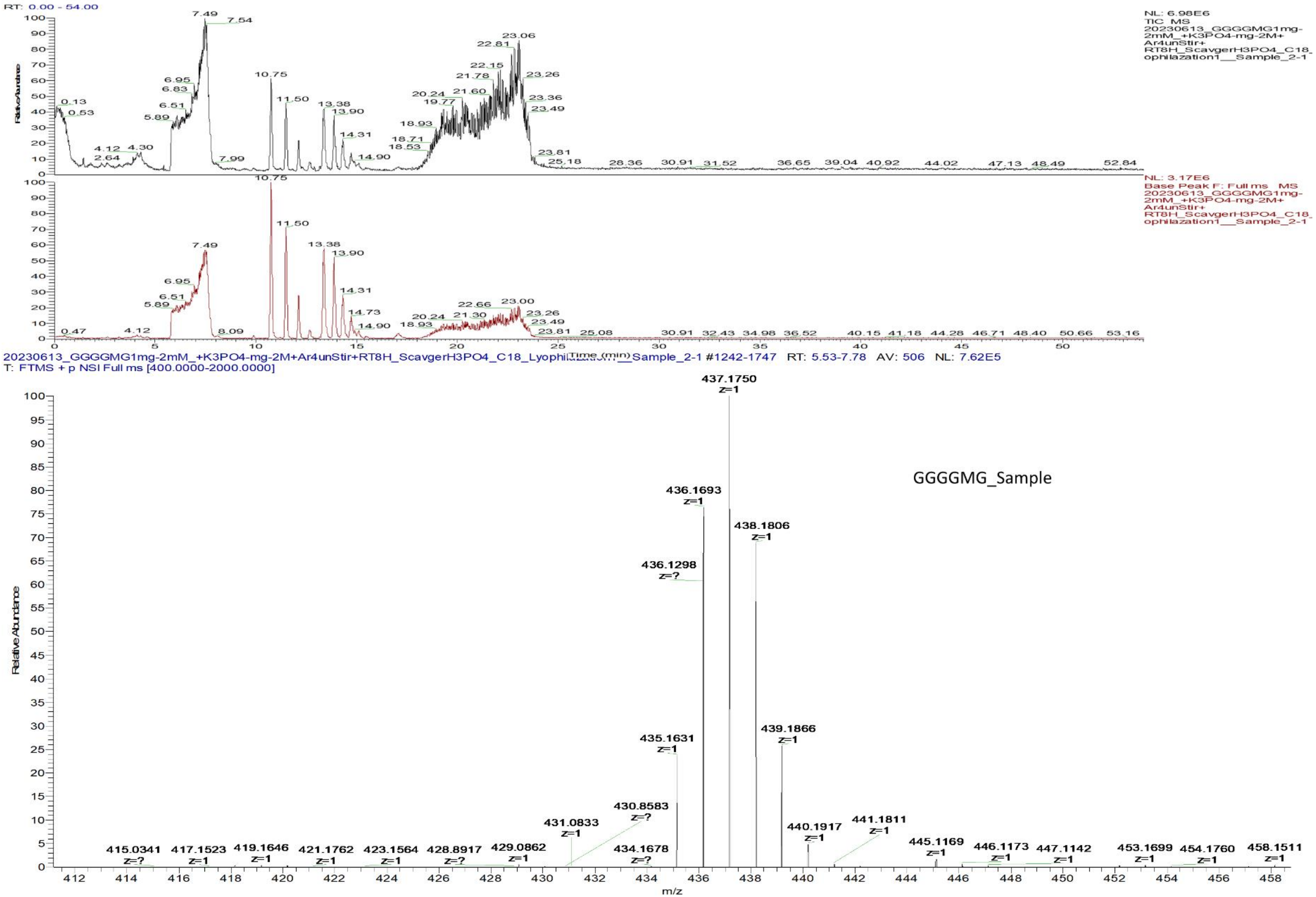
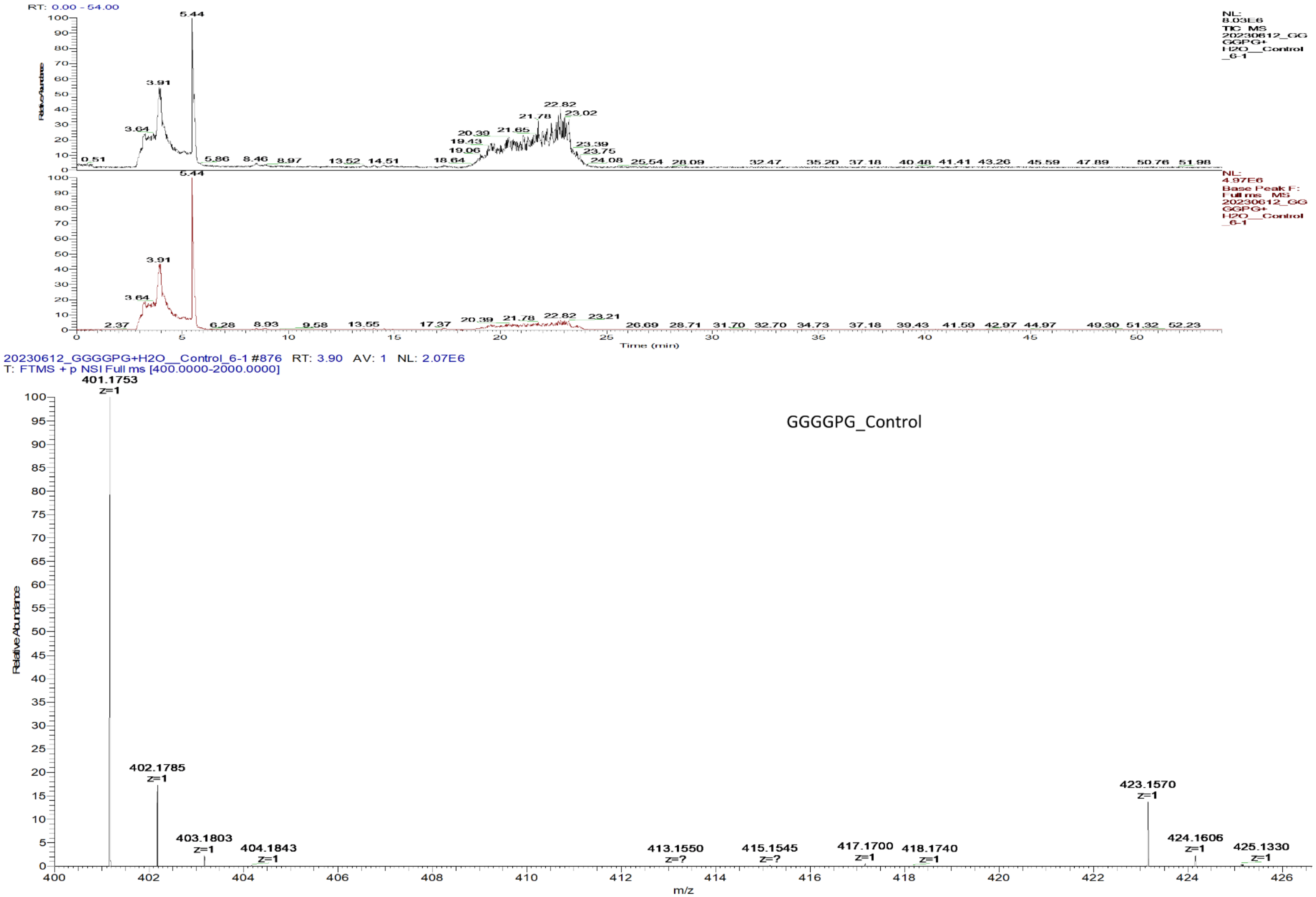
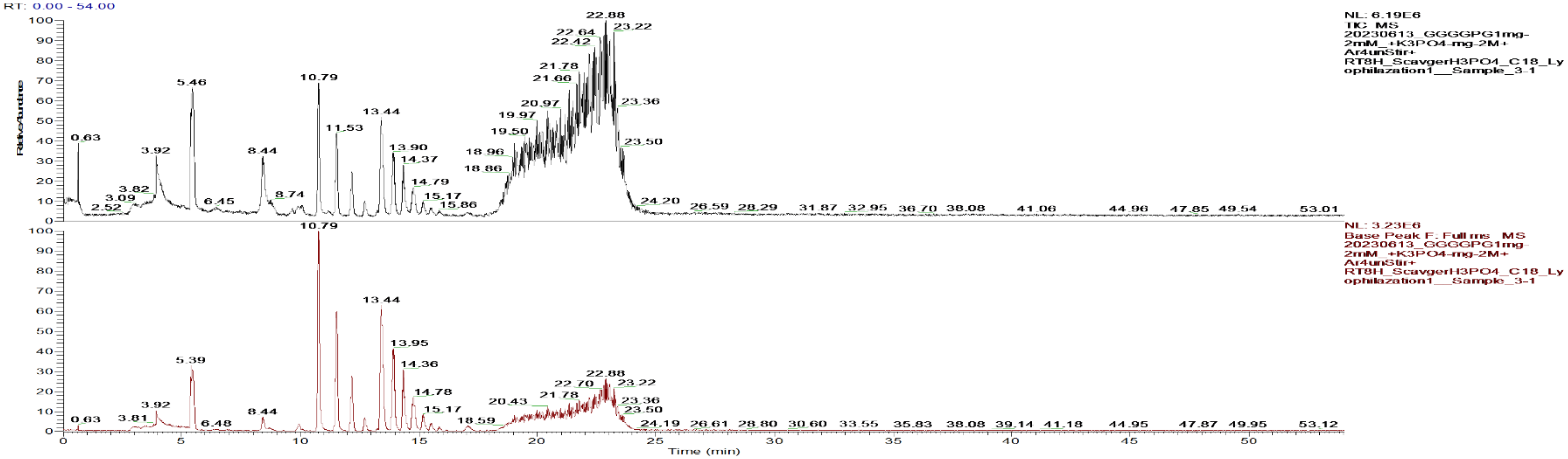
Relative Abundance
Time (min)

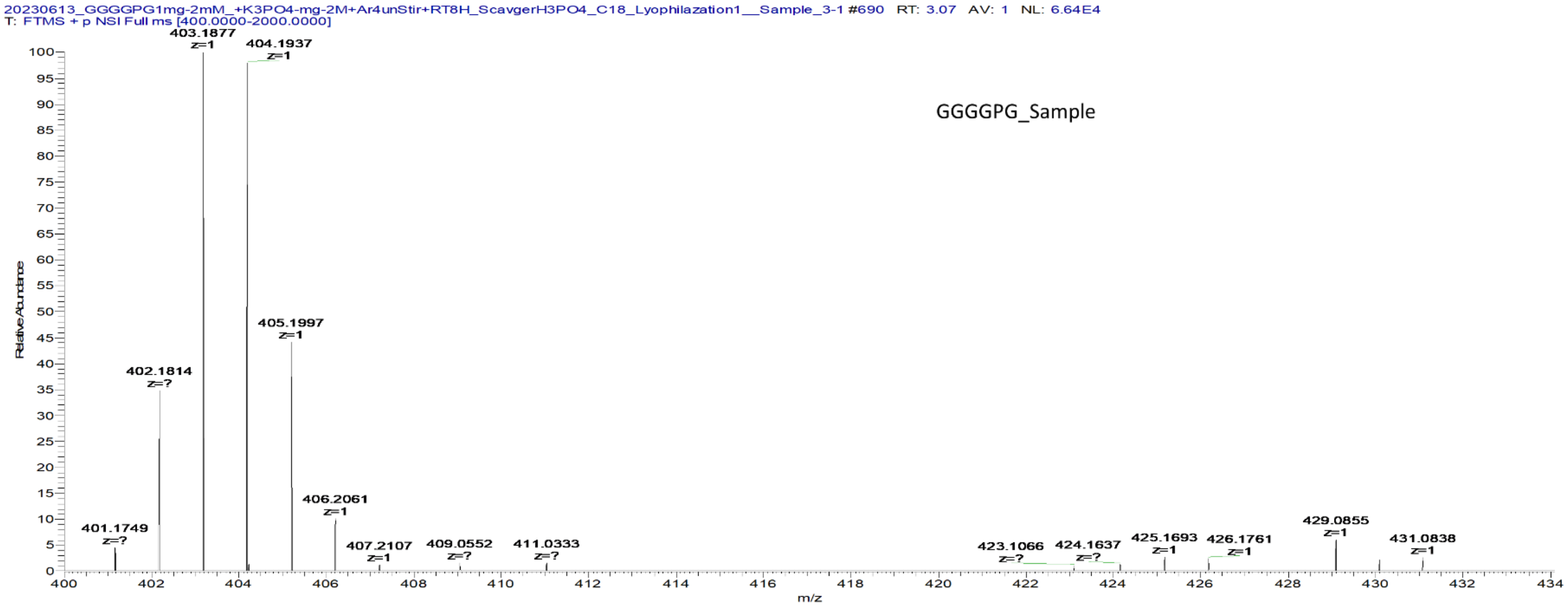

20230612_GGGGMG+H2O__Control_2-1 #1309-1844 RT: 5.83-8.22 AV: 536 NL: 2.51E6
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGMG_Control
435.1631
435.1058
436.1654
442.3940
443.1383
427.6934
434.9153
437.1584
Relative Abundance
m/z

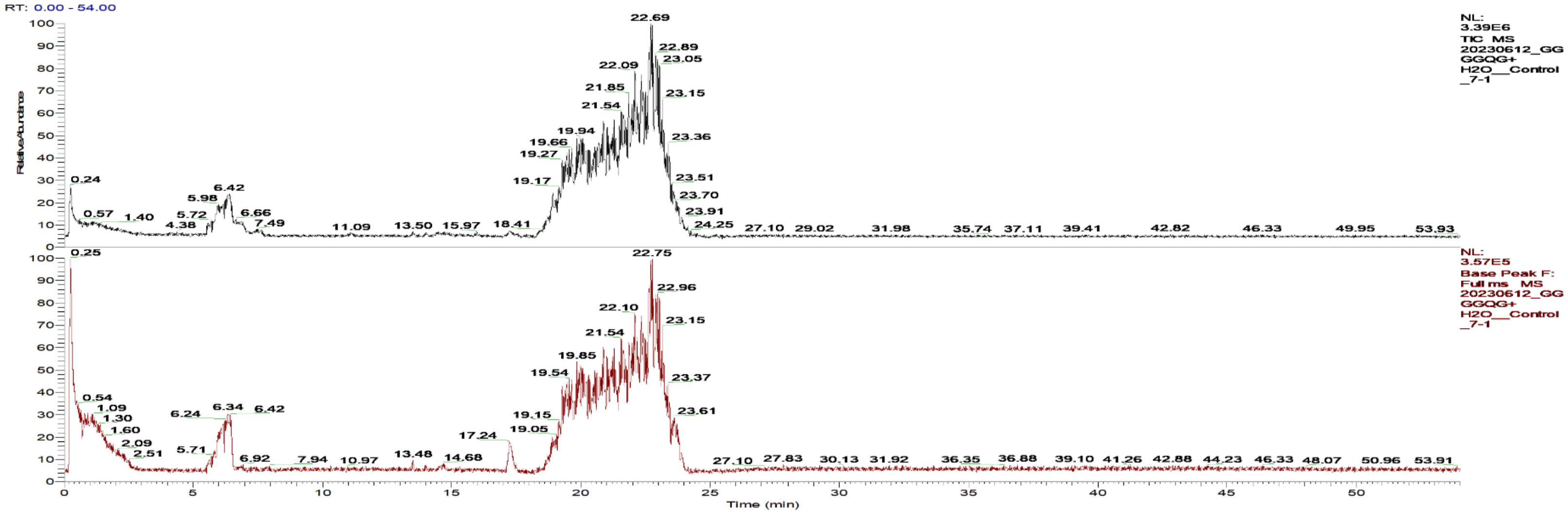


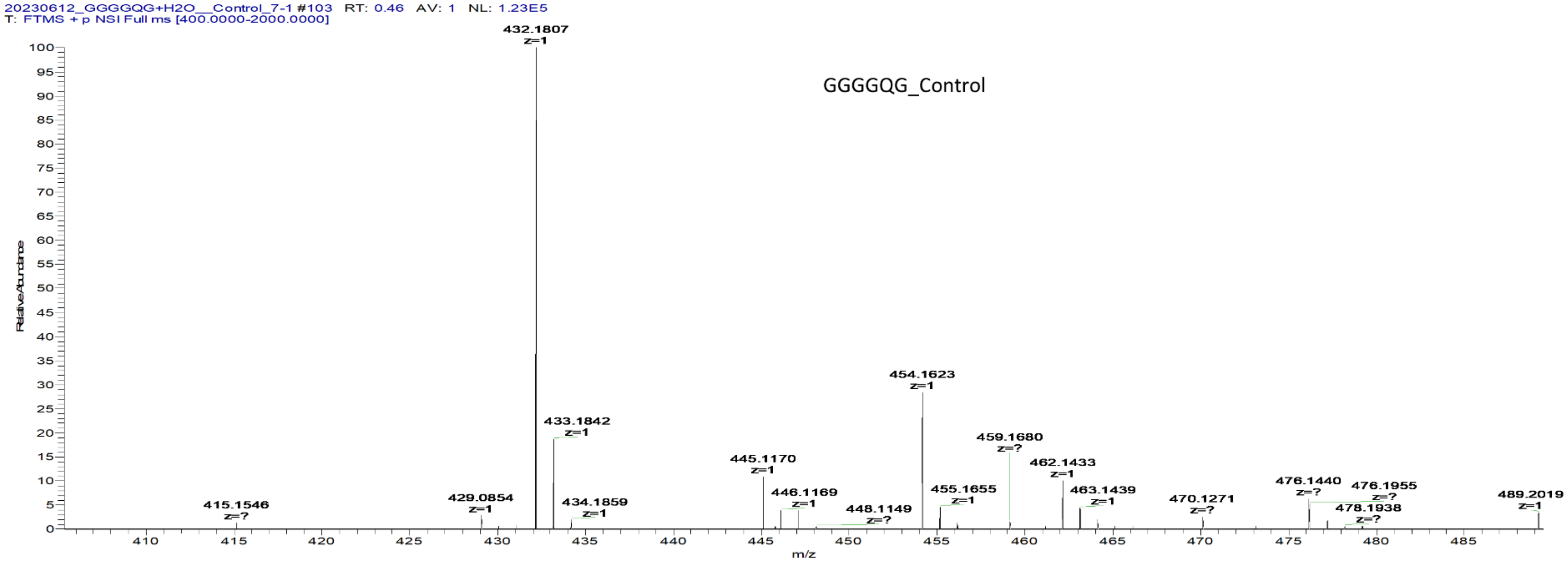
RT: 0.00 - 54.00
NL: 6.98E6
TIC MS
20230613_GGGGMG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_ophilazation1__Sample_2-1
NL: 3.17E6
Base Peak F: Full ms MS
20230613_GGGGMG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_ophilazation1__Sample_2-1
Relative Abundance
Time (min)
20230613_GGGGMG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophi...__Sample_2-1 #1242-1747 RT: 5.53-7.78 AV: 506 NL: 7.62E5
T: FTMS + p NSI Full ms [400.0000-2000.0000]
437.1750 z=1
436.1693 z=1
438.1806 z=1
436.1298 z=?
439.1866 z=1
435.1631 z=1
430.8583 z=?
431.0833 z=1
441.1811 z=1
440.1917 z=1
445.1169 z=1
GGGGMG_Sample
Relative Abundance
m/z

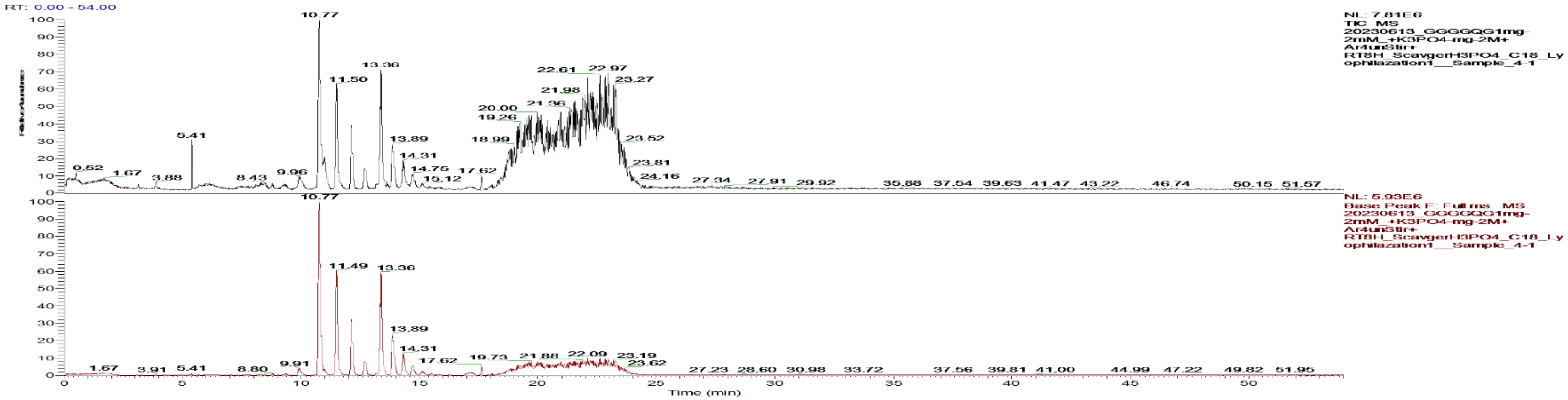

RT: 0.00 - 54.00
NL: 8.03E6 TIC MS 20230612_GGGGPG+H2O__Control_6-1
NL: 4.97E6 Base Peak F: Full ms MS 20230612_GGGGPG+H2O__Control_6-1
Relative Abundance
Time (min)
20230612_GGGGPG+H2O__Control_6-1 #876 RT: 3.90 AV: 1 NL: 2.07E6
T: FTMS + p NSI Full ms [400.0000-2000.0000]
401.1753 z=1
402.1785 z=1
403.1803 z=1
404.1843 z=1
413.1550 z=?
415.1545 z=?
417.1700 z=1
418.1740 z=1
423.1570 z=1
424.1606 z=1
425.1330 z=1
GGGGPG_Control
m/z

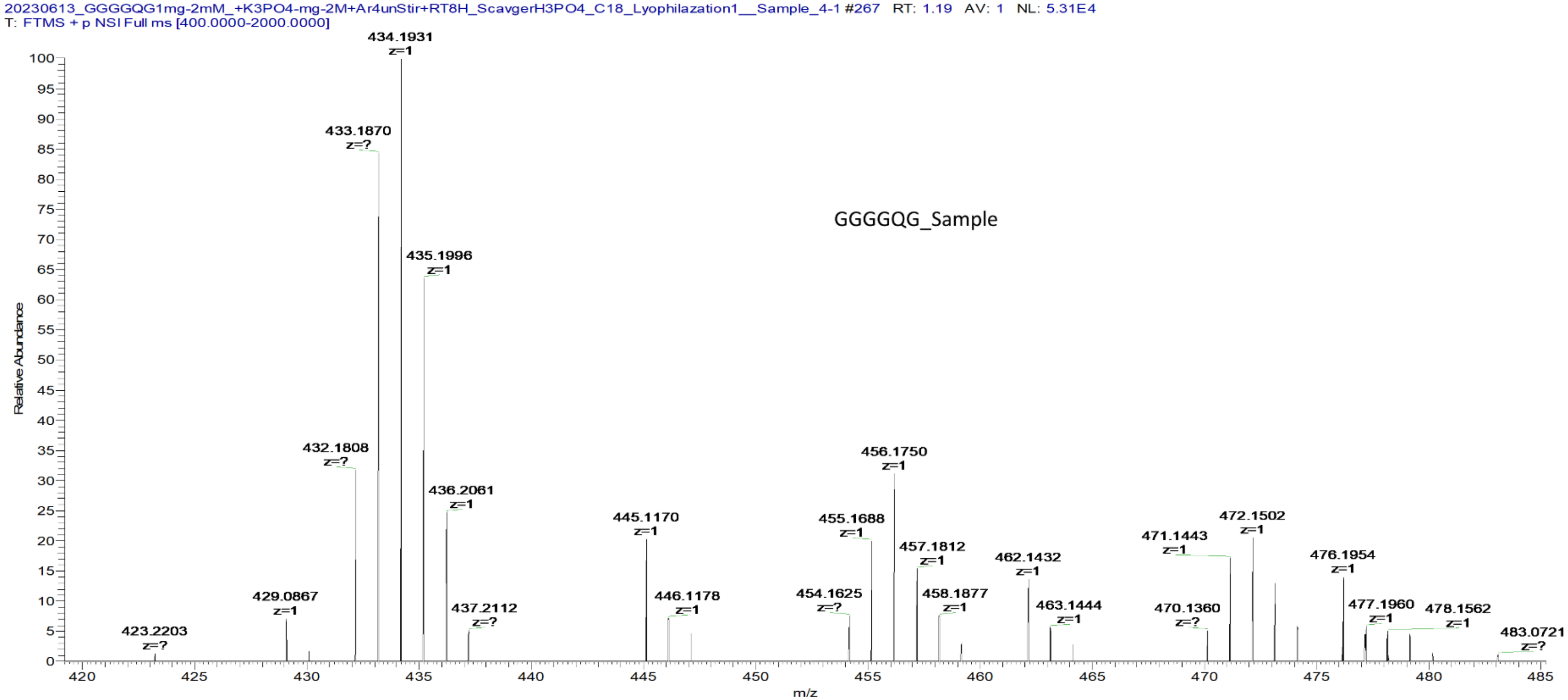

RT: 0.00 - 54.00
NL: 6.19E6
TIC MS
20230613_GGGGPG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1
NL: 3.23E6
Base Peak F: Full ms MS
20230613_GGGGPG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1
Relative Abundance
Time (min)

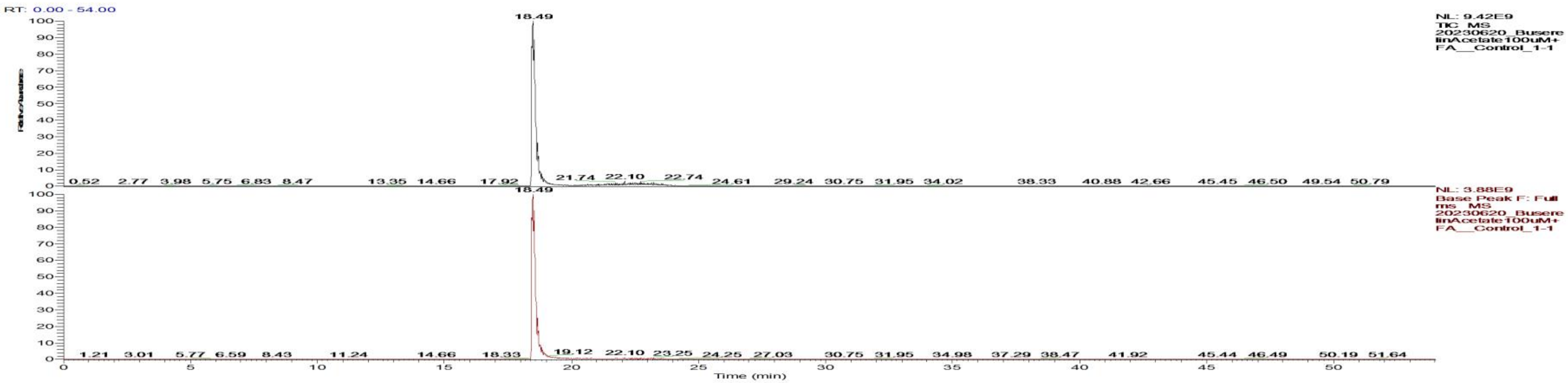

20230613_GGGGPG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1 #690 RT: 3.07 AV: 1 NL: 6.64E4
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGPG_Sample
Relative Abundance
m/z

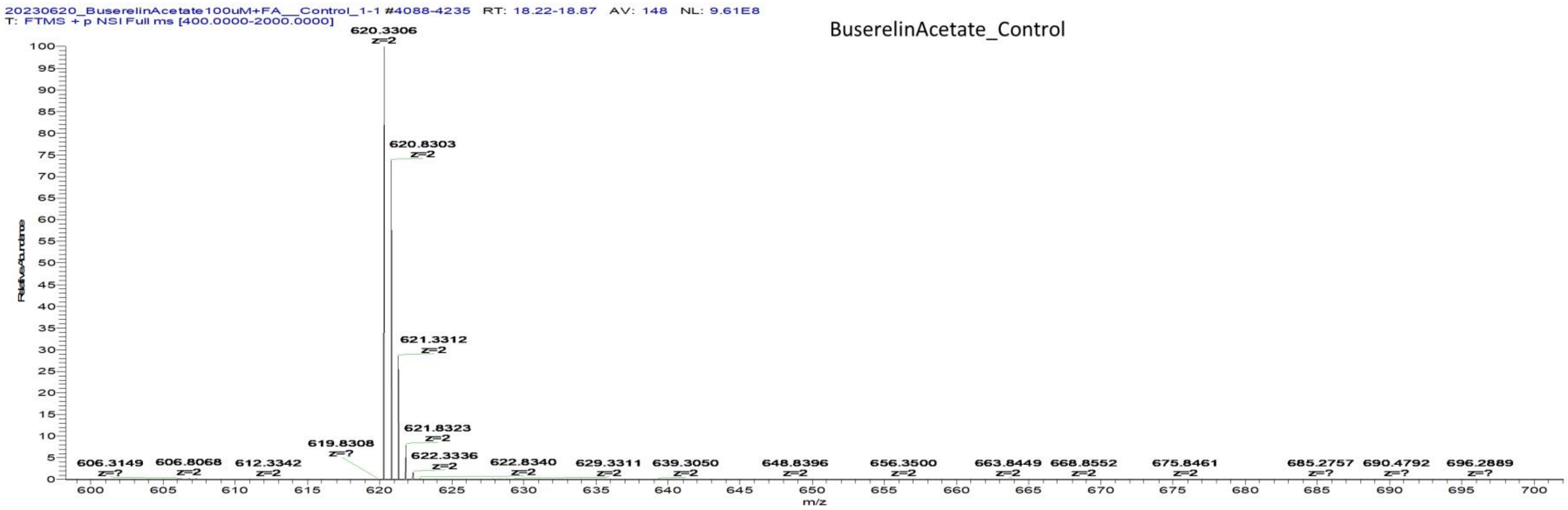

RT: 0.00 - 54.00
NL: 3.39E6 TIC MS 20230612_GGGGQG+H2O__Control_7-1
NL: 3.57E5 Base Peak F: Full ms MS 20230612_GGGGQG+H2O__Control_7-1
Relative Abundance
Time (min)

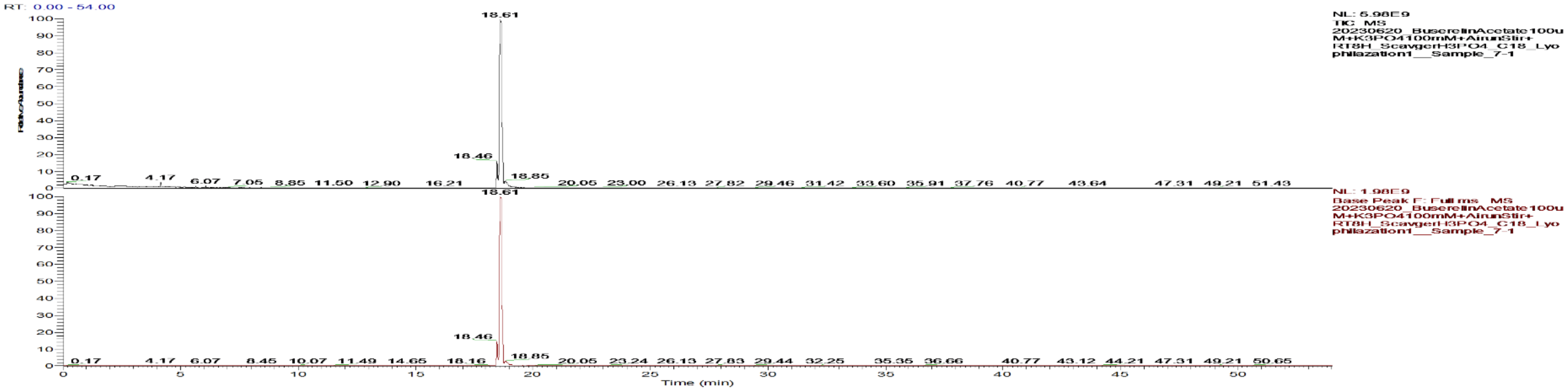

20230612_GGGGQG+H2O__Control_7-1 #103 RT: 0.46 AV: 1 NL: 1.23E5
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGQG_Control
432.1807 z=1
454.1623 z=1
433.1842 z=1
459.1680 z=?
445.1170 z=1
462.1433 z=1
Relative Abundance
m/z

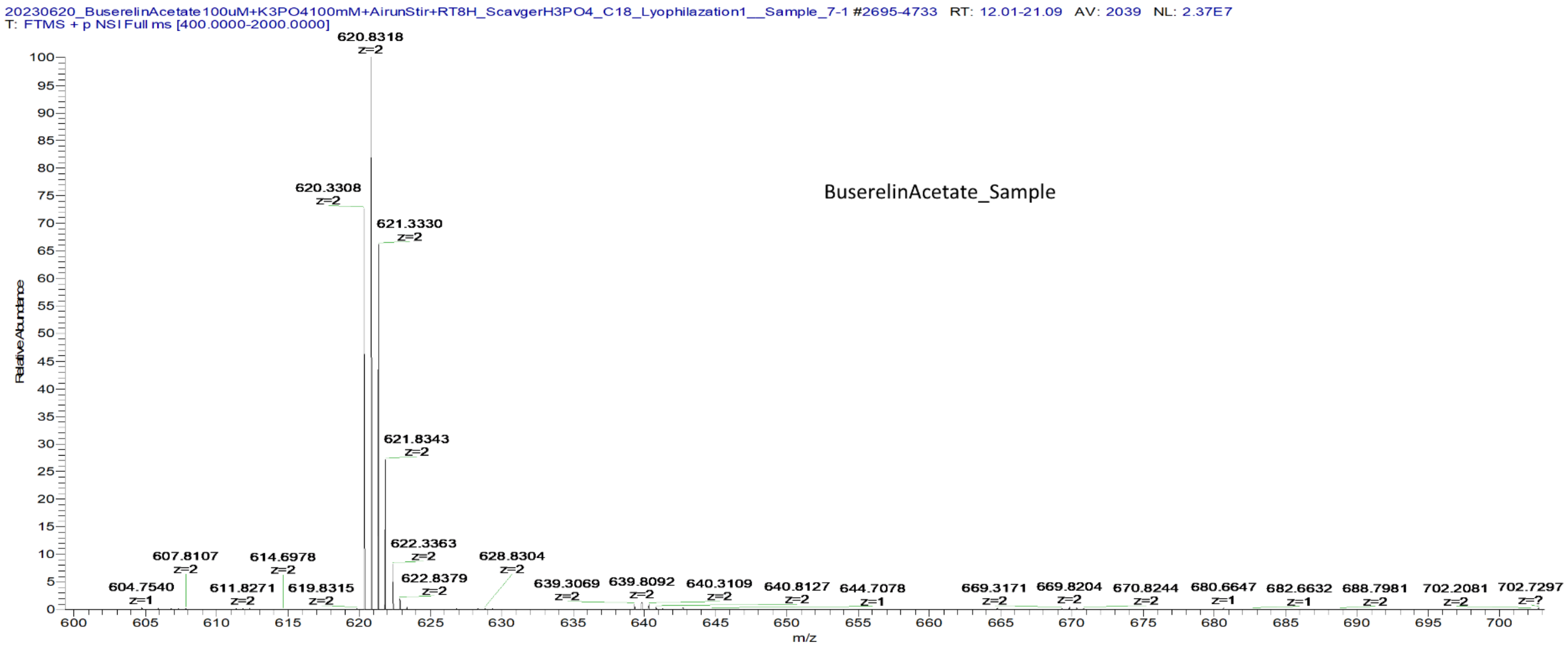

RT: 0.00 - 54.00
NL: 7.81E6
TIC MS
20230613_GGGGQG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_4-1
NL: 5.93E6
Base Peak F: Full ms MS
20230613_GGGGQG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_4-1
Time (min)

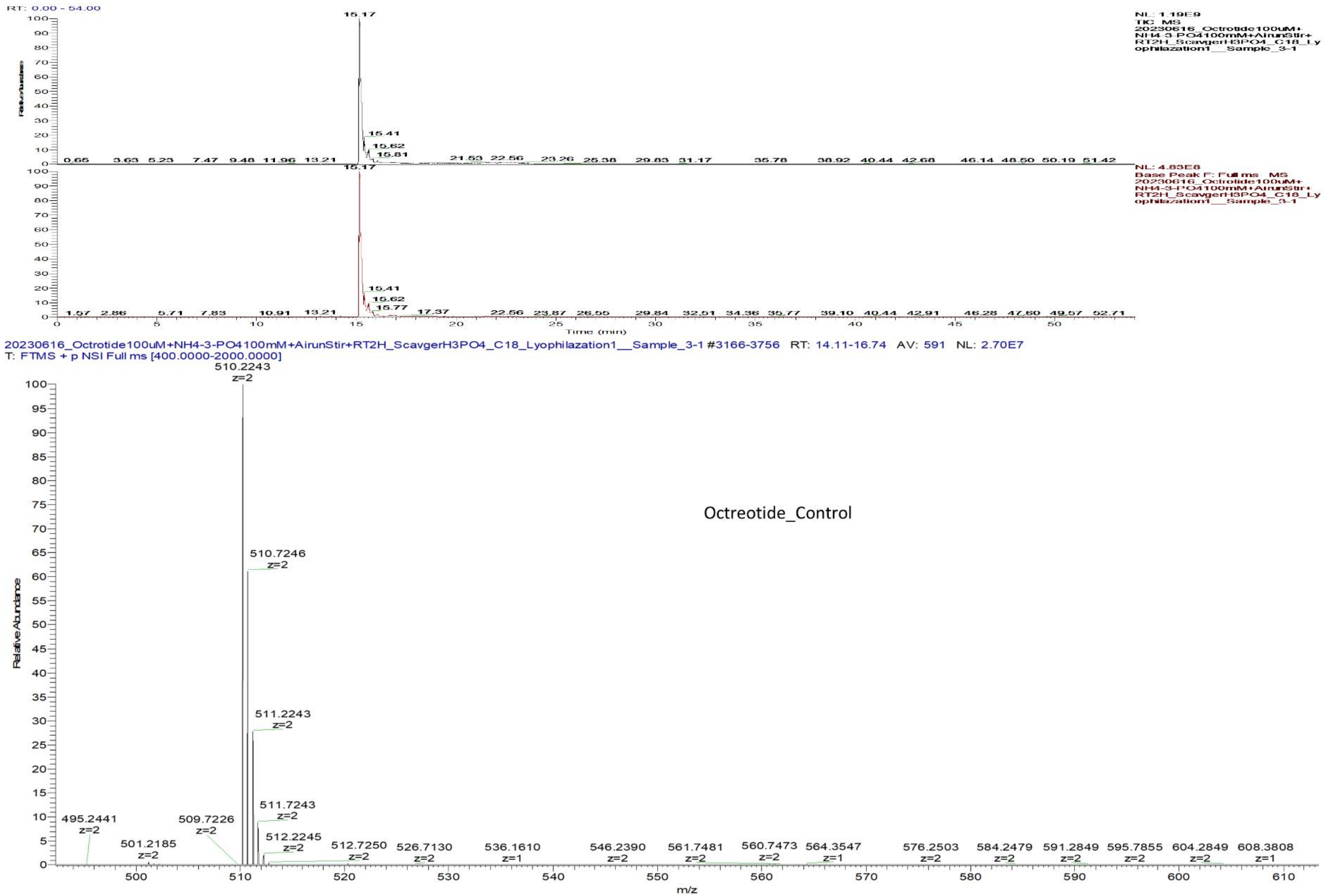

20230613_GGGGQG1mg-2mM_+K3PO4-mg-2M+Ar4unStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_4-1 #267 RT: 1.19 AV: 1 NL: 5.31E4
T: FTMS + p NSI Full ms [400.0000-2000.0000]
GGGGQG_Sample
Relative Abundance
m/z
434.1931 z=1
433.1870 z=?
435.1996 z=1
432.1808 z=?
436.2061 z=1
456.1750 z=1
445.1170 z=1
455.1688 z=1
472.1502 z=1
471.1443 z=1
457.1812 z=1
462.1432 z=1
476.1954 z=1
429.0867 z=1
446.1178 z=1
454.1625 z=?
458.1877 z=1
463.1444 z=1
470.1360 z=?
477.1960 z=1
478.1562 z=1
437.2112 z=?
423.2203 z=?
483.0721 z=?

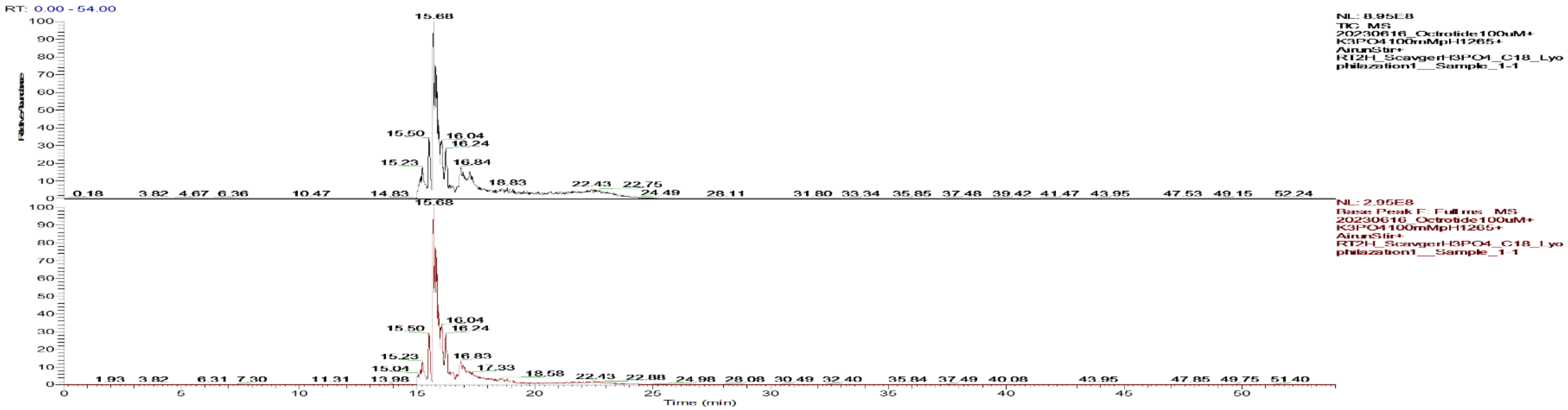

RT: 0.00 - 54.00
NL: 9.42E9
TIC MS
20230620_BuserelinAcetate100uM+FA__Control_1-1
NL: 3.88E9
Base Peak F: Full ms MS
20230620_BuserelinAcetate100uM+FA__Control_1-1
Relative Abundance
Time (min)
18.49

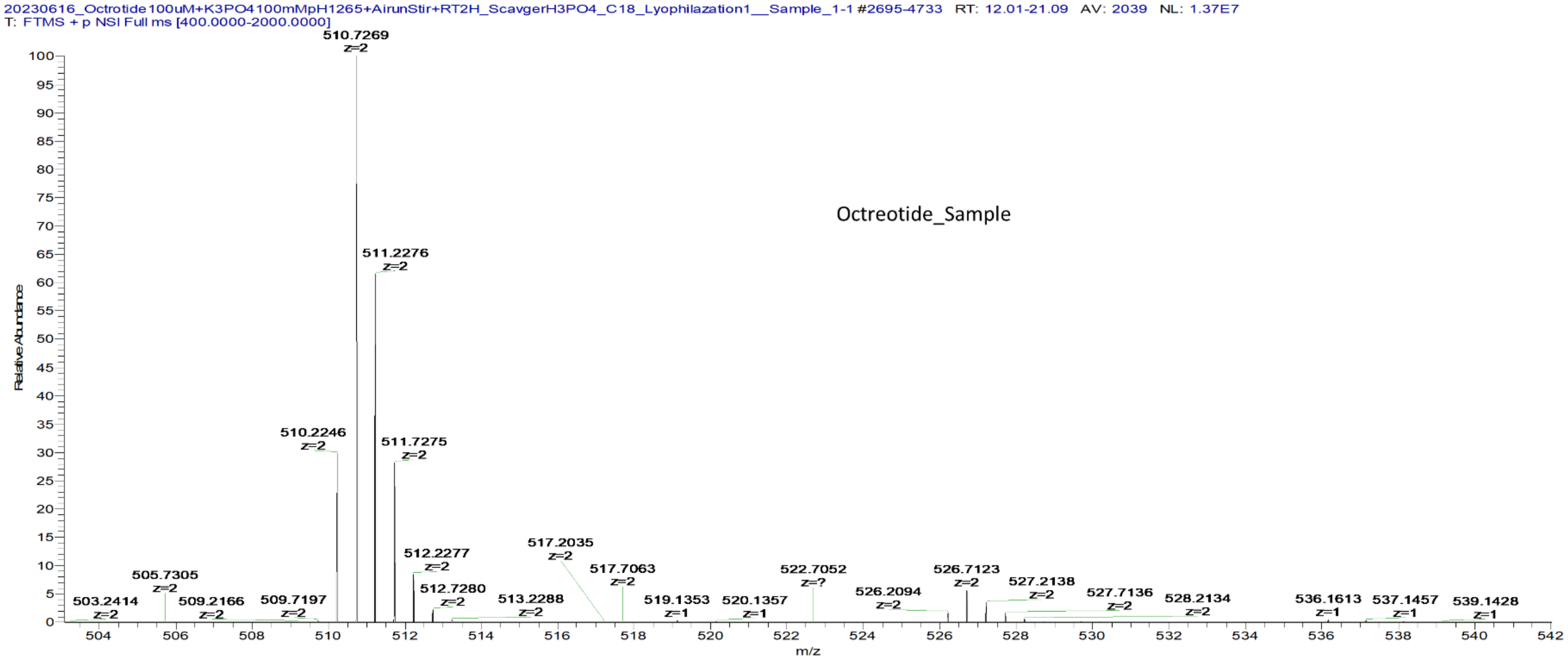

20230620_BuserelinAcetate100uM+FA__Control_1-1 #4088-4235 RT: 18.22-18.87 AV: 148 NL: 9.61E8
T: FTMS + p NSI Full ms [400.0000-2000.0000]
BuserelinAcetate_Control
620.3306 z=2
620.8303 z=2
621.3312 z=2
621.8323 z=2
622.3336 z=2
619.8308 z=?
Relative Abundance
m/z

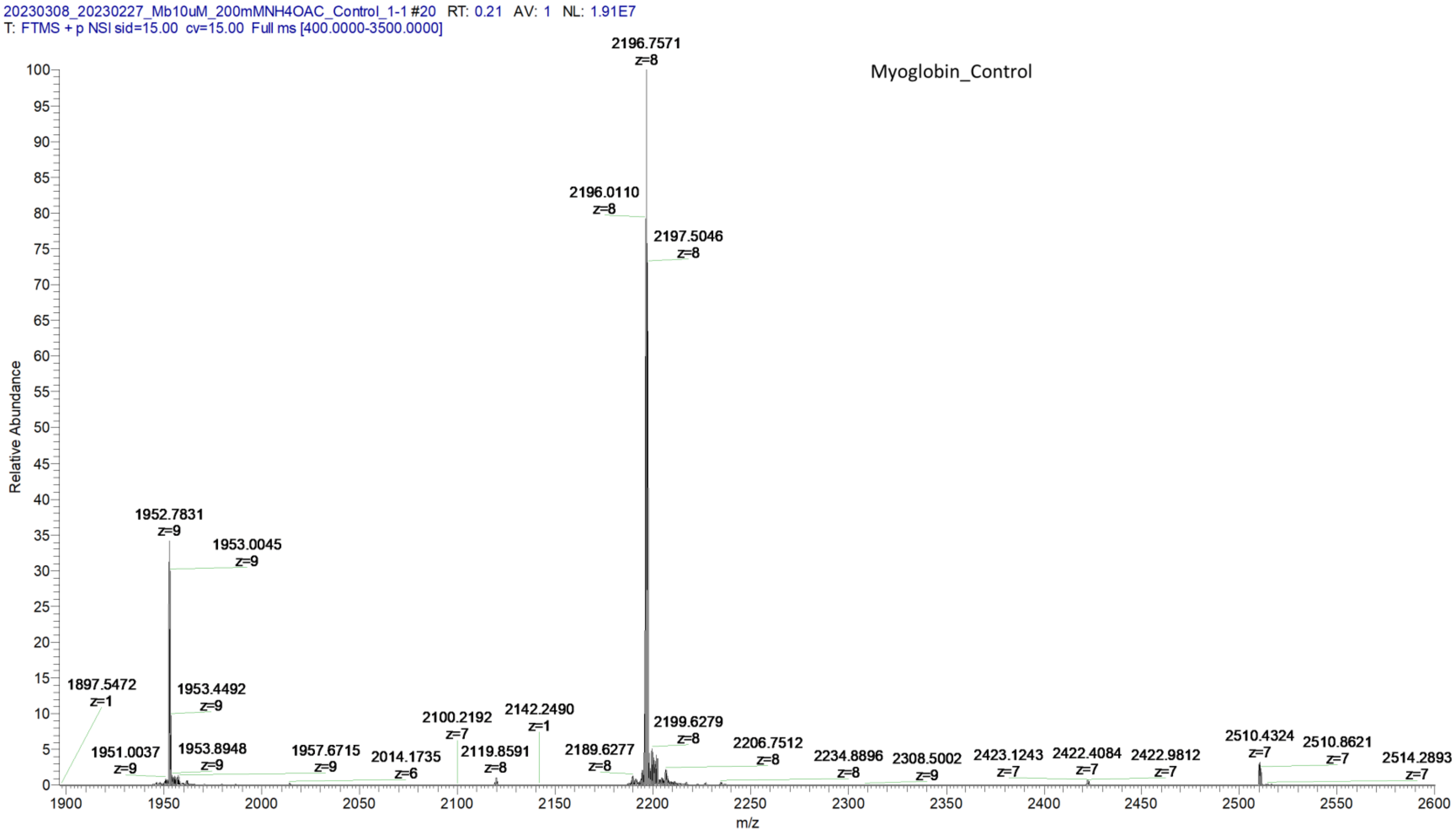

RT: 0.00 - 54.00
NL: 5.98E9
TIC MS
20230620_BuserelinAcetate100uM+K3PO4100mM+AirunStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_7-1
NL: 1.98E9
Base Peak F: Full ms MS
20230620_BuserelinAcetate100uM+K3PO4100mM+AirunStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_7-1
18.61
18.46
18.85
Time (min)

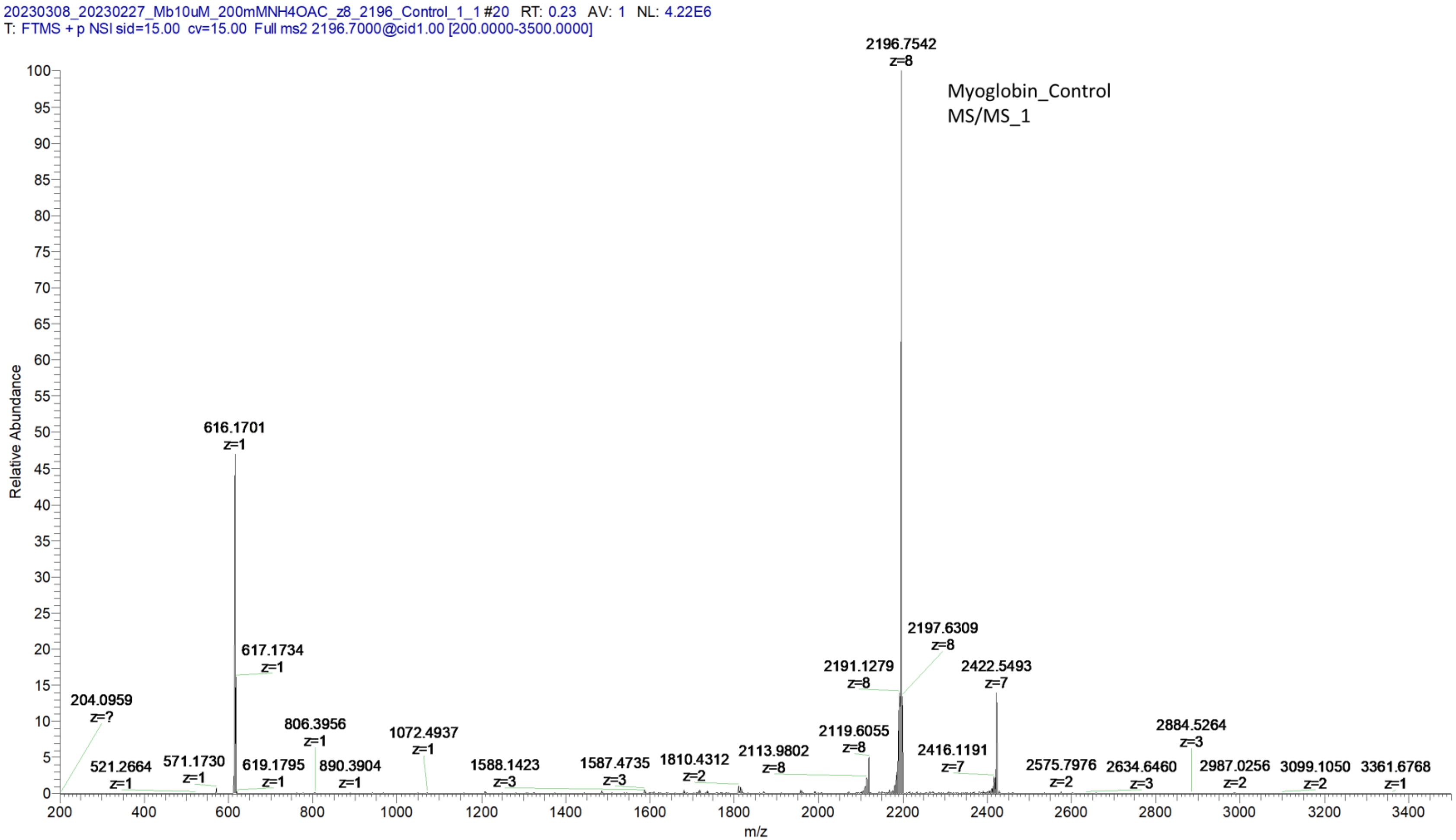

20230620_BuserelinAcetate100uM+K3PO4100mM+AirunStir+RT8H_ScavgerH3PO4_C18_Lyophilazation1__Sample_7-1 #2695-4733 RT: 12.01-21.09 AV: 2039 NL: 2.37E7
T: FTMS + p NSI Full ms [400.0000-2000.0000]
BuserelinAcetate_Sample
620.8318 z=2
620.3308 z=2
621.3330 z=2
621.8343 z=2
622.3363 z=2
622.8379 z=2
628.8304 z=2
607.8107 z=2
614.6978 z=2
604.7540 z=1
611.8271 z=2
619.8315 z=2
639.3069 z=2
639.8092 z=2
640.3109 z=2
640.8127 z=2
644.7078 z=1
669.3171 z=2
669.8204 z=2
670.8244 z=2
680.6647 z=1
682.6632 z=1
688.7981 z=2
702.2081 z=2
702.7297 z=?
Relative Abundance
m/z

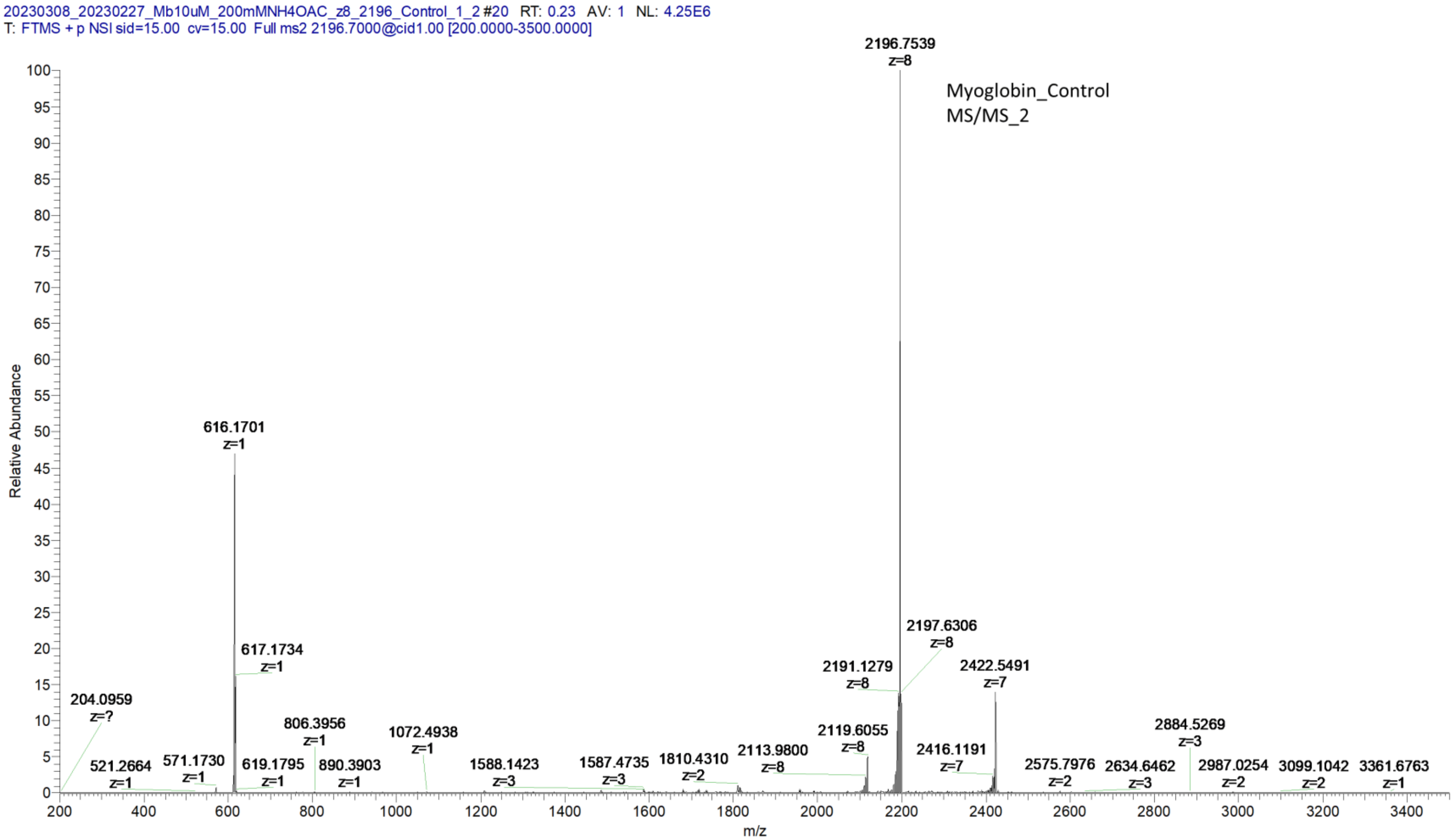

RT: 0.00 - 54.00
NL: 1.19E9
TIC MS
20230616_Octrotide100uM+NH4-3-PO4100mM+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1
NL: 4.83E8
Base Peak F: Full ms MS
20230616_Octrotide100uM+NH4-3-PO4100mM+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1
Time (min)
20230616_Octrotide100uM+NH4-3-PO4100mM+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_3-1 #3166-3756 RT: 14.11-16.74 AV: 591 NL: 2.70E7
T: FTMS + p NSI Full ms [400.0000-2000.0000]
510.2243 z=2
510.7246 z=2
511.2243 z=2
511.7243 z=2
512.2245 z=2
495.2441 z=2
501.2185 z=2
509.7226 z=2
512.7250 z=2
526.7130 z=2
536.1610 z=1
546.2390 z=2
561.7481 z=2
560.7473 z=2
564.3547 z=1
576.2503 z=2
584.2479 z=2
591.2849 z=2
595.7855 z=2
604.2849 z=2
608.3808 z=1
Octreotide_Control
Relative Abundance
m/z

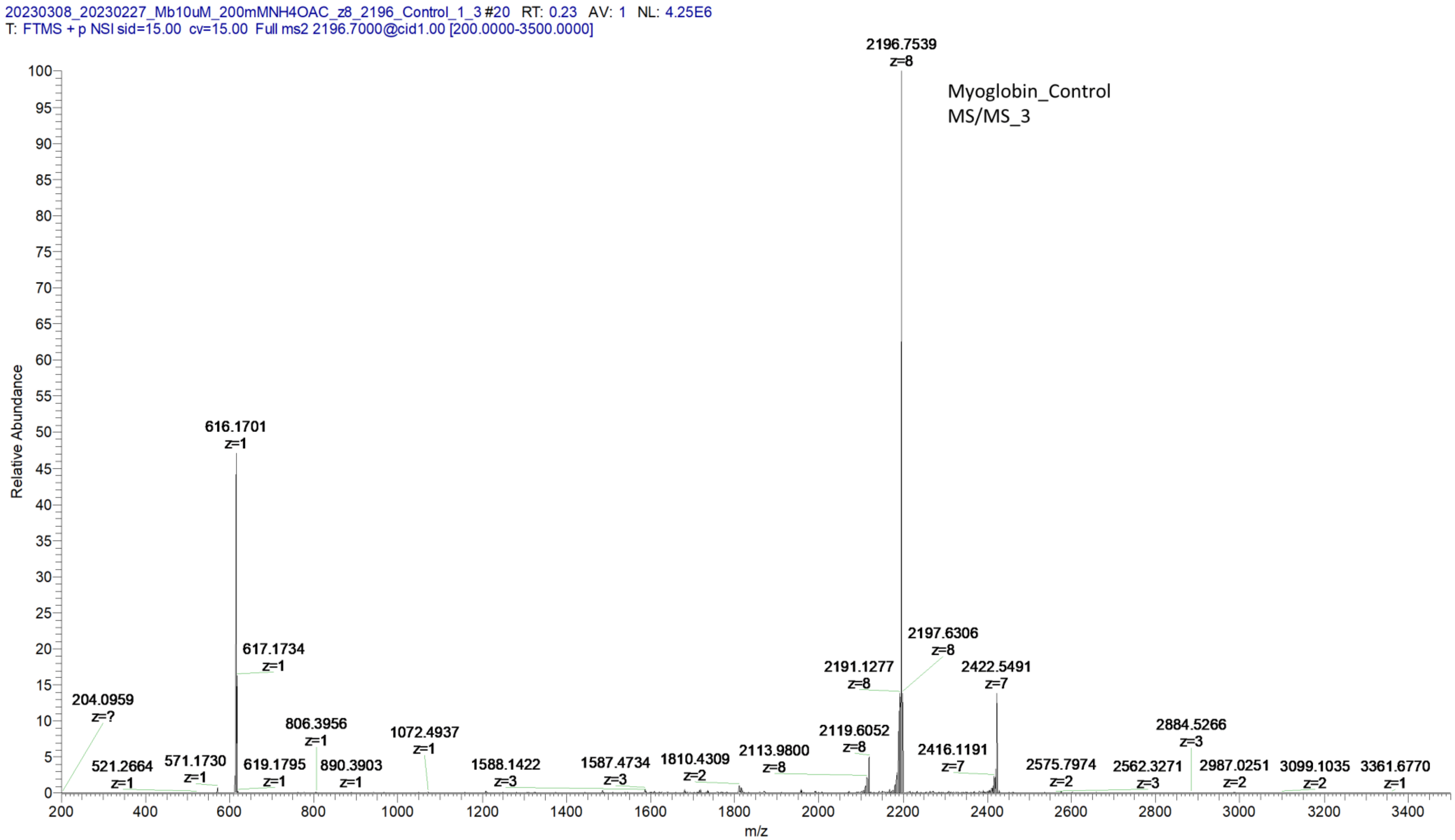

RT: 0.00 - 54.00
NL: 8.95E8
TIC MS
20230616_Octrotide100uM+K3PO4100mMpH1265+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1
NL: 2.95E8
Base Peak F: Full ms MS
20230616_Octrotide100uM+K3PO4100mMpH1265+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1
Relative Abundance
Time (min)

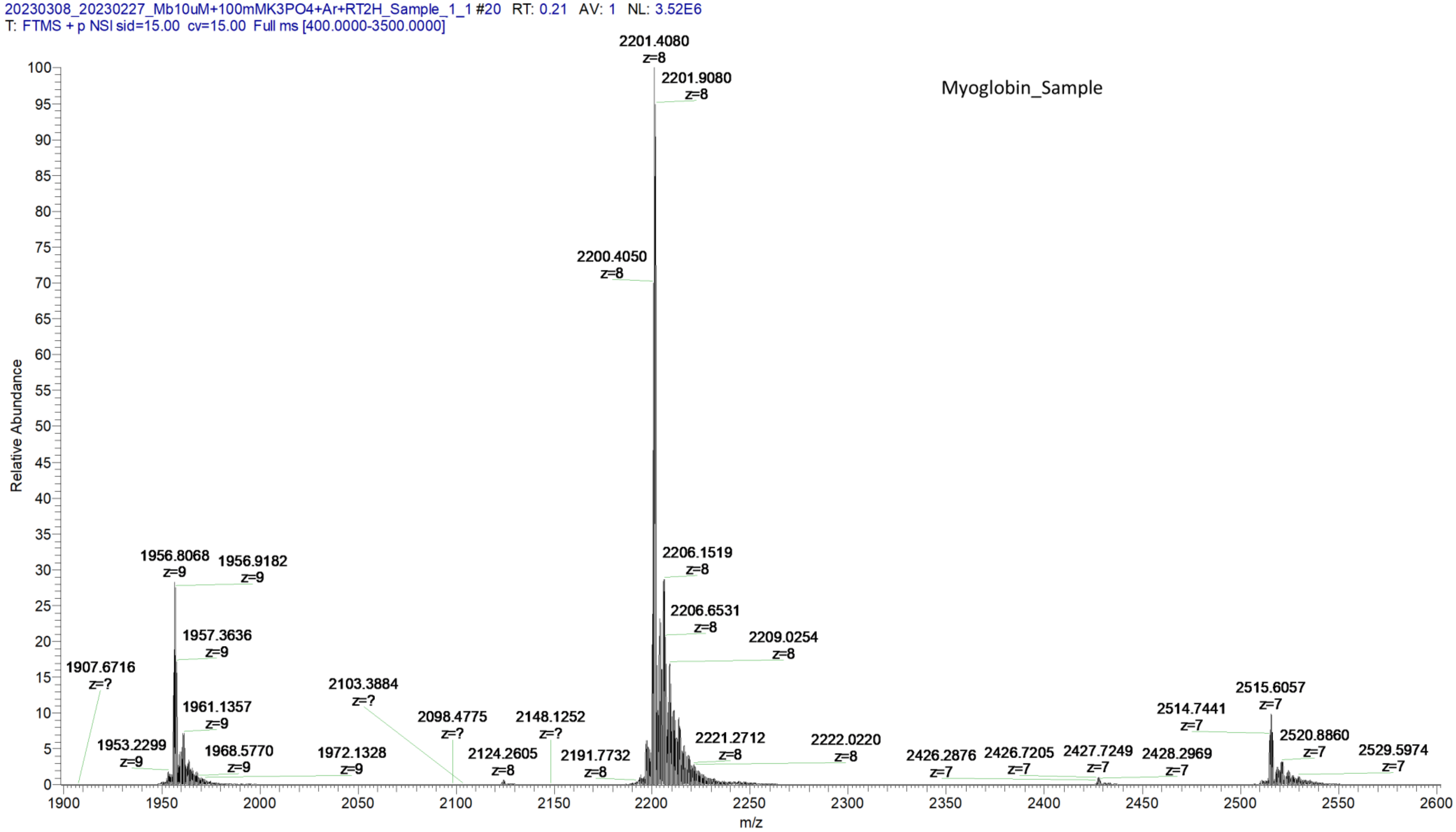

20230616_Octrotide100uM+K3PO4100mMpH1265+AirunStir+RT2H_ScavgerH3PO4_C18_Lyophilazation1__Sample_1-1 #2695-4733 RT: 12.01-21.09 AV: 2039 NL: 1.37E7
T: FTMS + p NSI Full ms [400.0000-2000.0000]
510.7269 z=2
511.2276 z=2
510.2246 z=2
511.7275 z=2
512.2277 z=2
512.7280 z=2
517.2035 z=2
517.7063 z=2
505.7305 z=2
503.2414 z=2
509.2166 z=2
509.7197 z=2
513.2288 z=2
519.1353 z=1
520.1357 z=1
522.7052 z=?
526.2094 z=2
526.7123 z=2
527.2138 z=2
527.7136 z=2
528.2134 z=2
536.1613 z=1
537.1457 z=1
539.1428 z=1
Octreotide_Sample
Relative Abundance
m/z

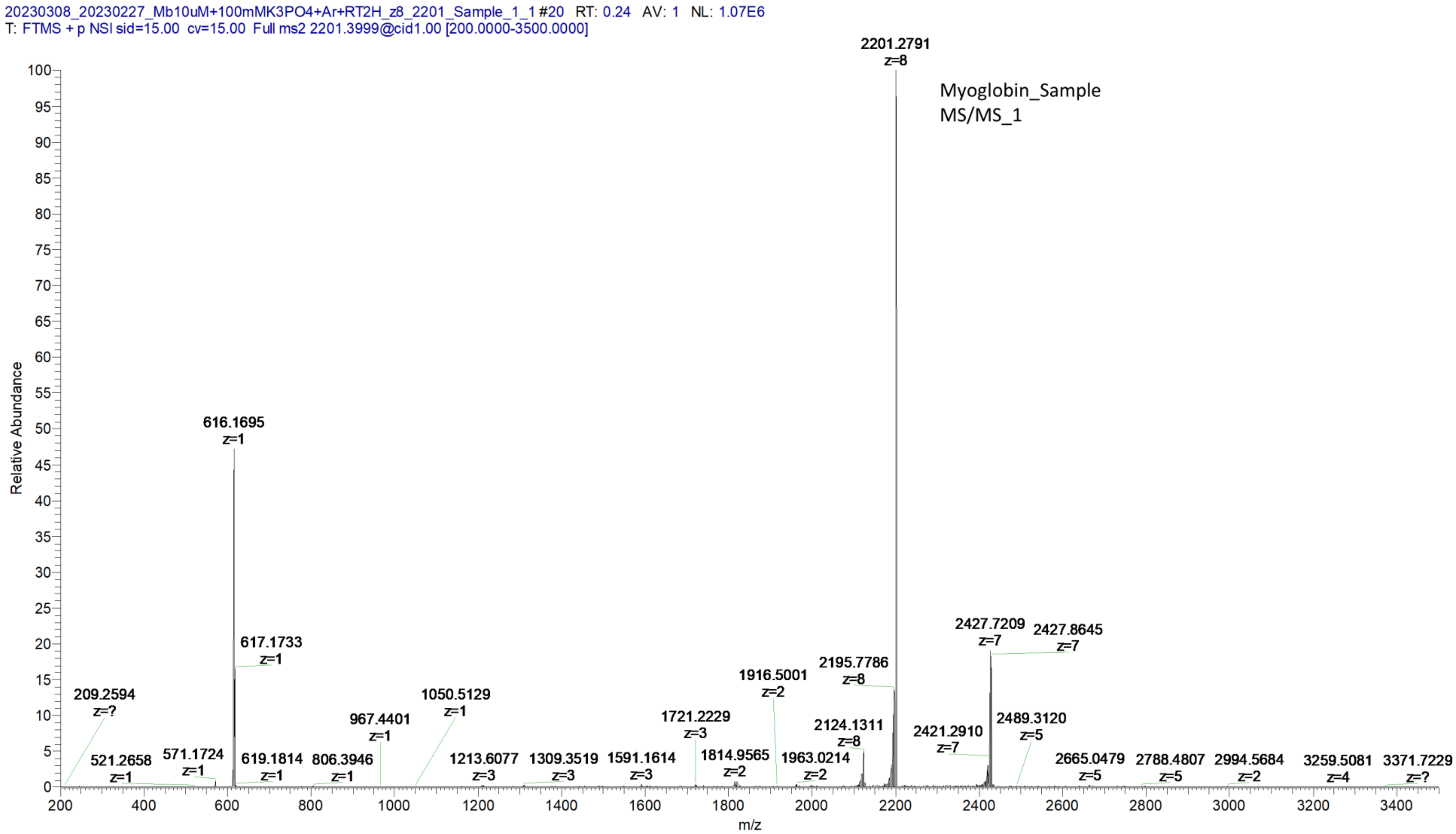

20230308_20230227_Mb10uM_200mMNH4OAC_Control_1-1 #20 RT: 0.21 AV: 1 NL: 1.91E7
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms [400.0000-3500.0000]
Myoglobin_Control
2196.7571 z=8
2196.0110 z=8
2197.5046 z=8
1952.7831 z=9
1953.0045 z=9
1897.5472 z=1
1953.4492 z=9
1951.0037 z=9
1953.8948 z=9
1957.6715 z=9
2014.1735 z=6
2100.2192 z=7
2119.8591 z=8
2142.2490 z=1
2189.6277 z=8
2199.6279 z=8
2206.7512 z=8
2234.8896 z=8
2308.5002 z=9
2423.1243 z=7
2422.4084 z=7
2422.9812 z=7
2510.4324 z=7
2510.8621 z=7
2514.2893 z=7
Relative Abundance
m/z

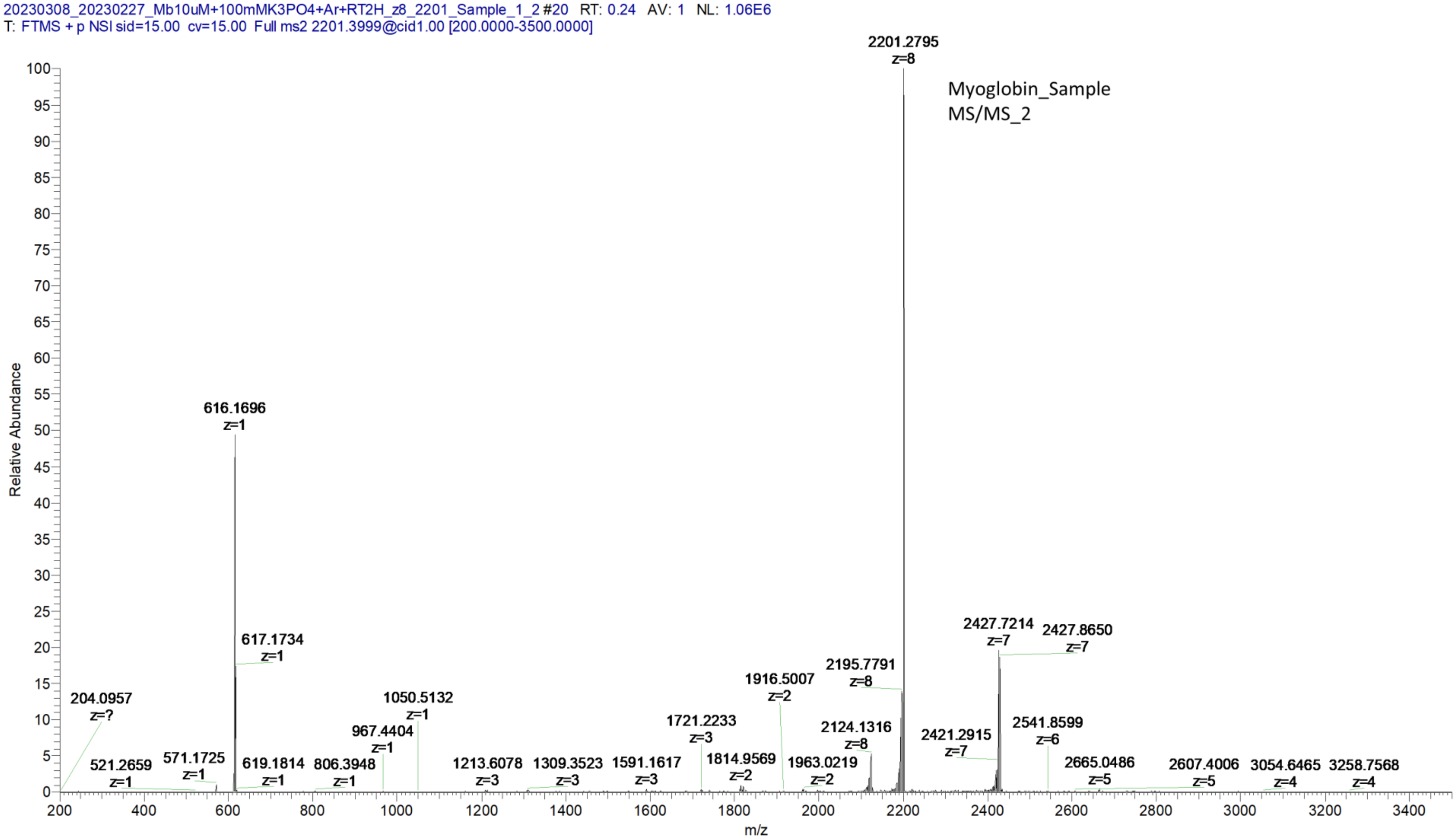

20230308_20230227_Mb10uM_200mMNH4OAC_z8_2196_Control_1_1 #20 RT: 0.23 AV: 1 NL: 4.22E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2196.7000@cid1.00 [200.0000-3500.0000]
Myoglobin_Control
MS/MS_1
Relative Abundance
m/z
2196.7542 z=8
616.1701 z=1
617.1734 z=1
204.0959 z=?
521.2664 z=1
571.1730 z=1
619.1795 z=1
806.3956 z=1
890.3904 z=1
1072.4937 z=1
1588.1423 z=3
1587.4735 z=3
1810.4312 z=2
2113.9802 z=8
2119.6055 z=8
2191.1279 z=8
2197.6309 z=8
2416.1191 z=7
2422.5493 z=7
2575.7976 z=2
2634.6460 z=3
2884.5264 z=3
2987.0256 z=2
3099.1050 z=2
3361.6768 z=1

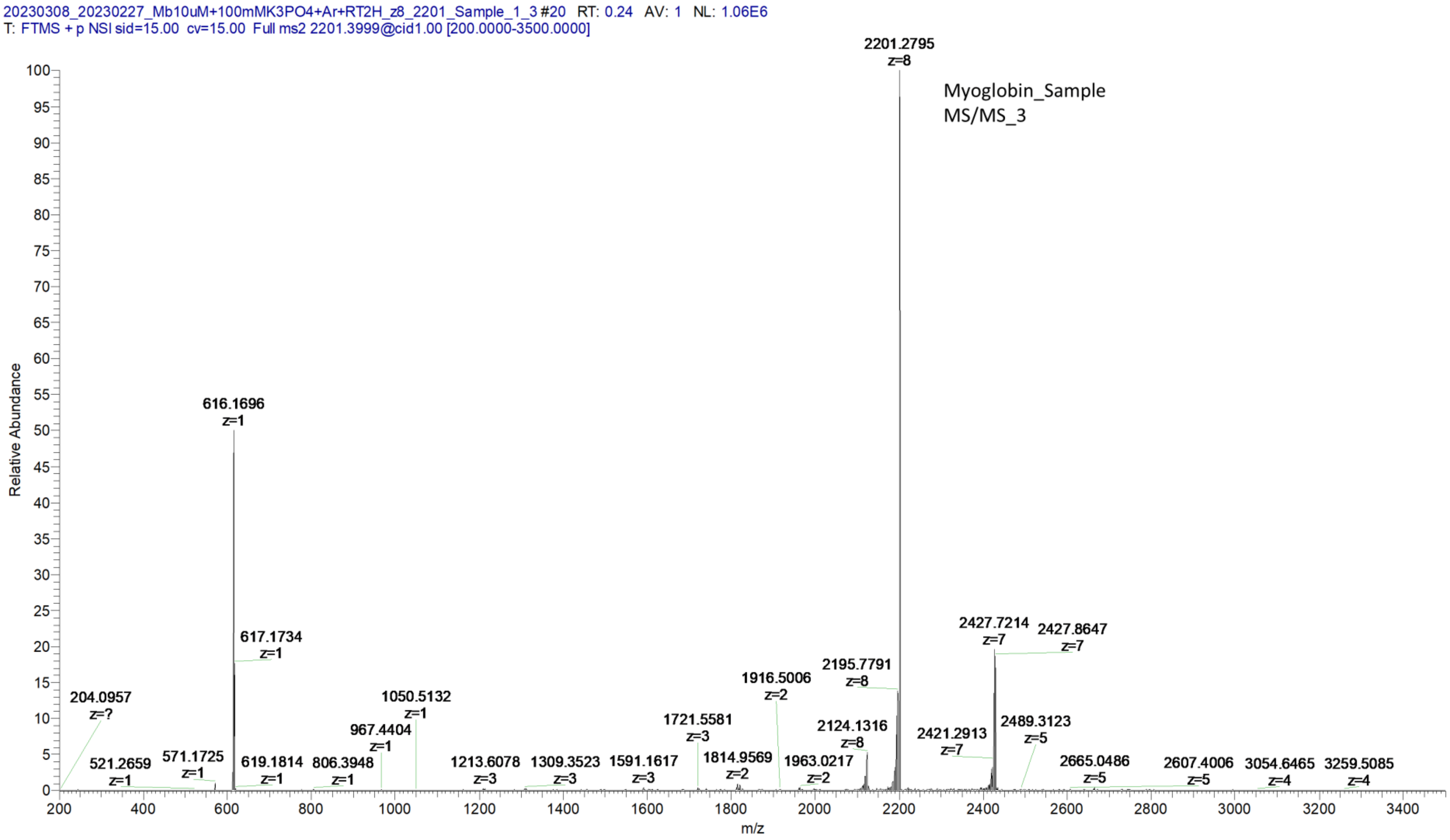

20230308_20230227_Mb10uM_200mMNH4OAC_z8_2196_Control_1_2 #20 RT: 0.23 AV: 1 NL: 4.25E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2196.7000@cid1.00 [200.0000-3500.0000]
Myoglobin_Control
MS/MS_2
Relative Abundance
m/z
2196.7539 z=8
616.1701 z=1
617.1734 z=1
204.0959 z=?
521.2664 z=1
571.1730 z=1
619.1795 z=1
806.3956 z=1
890.3903 z=1
1072.4938 z=1
1588.1423 z=3
1587.4735 z=3
1810.4310 z=2
2113.9800 z=8
2119.6055 z=8
2191.1279 z=8
2197.6306 z=8
2416.1191 z=7
2422.5491 z=7
2575.7976 z=2
2634.6462 z=3
2884.5269 z=3
2987.0254 z=2
3099.1042 z=2
3361.6763 z=1


20230308_20230227_Mb10uM_200mMNH4OAC_z8_2196_Control_1_3 #20 RT: 0.23 AV: 1 NL: 4.25E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2196.7000@cid1.00 [200.0000-3500.0000]
Myoglobin_Control
MS/MS_3
Relative Abundance
m/z
2196.7539 z=8
616.1701 z=1
617.1734 z=1
2197.6306 z=8
2191.1277 z=8
2422.5491 z=7
204.0959 z=?
806.3956 z=1
1072.4937 z=1
2884.5266 z=3
2119.6052 z=8
2113.9800 z=8
2416.1191 z=7
1810.4309 z=2
521.2664 z=1
571.1730 z=1
619.1795 z=1
890.3903 z=1
1588.1422 z=3
1587.4734 z=3
2575.7974 z=2
2562.3271 z=3
2987.0251 z=2
3099.1035 z=2
3361.6770 z=1


20230308_20230227_Mb10uM+100mMK3PO4+Ar+RT2H_Sample_1_1 #20 RT: 0.21 AV: 1 NL: 3.52E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms [400.0000-3500.0000]
Myoglobin_Sample
Relative Abundance
m/z
2201.4080 z=8
2201.9080 z=8
2200.4050 z=8
2206.1519 z=8
2206.6531 z=8
2209.0254 z=8
2221.2712 z=8
2222.0220 z=8
2191.7732 z=8
2124.2605 z=8
2148.1252 z=?
2098.4775 z=?
2103.3884 z=?
1956.8068 z=9
1956.9182 z=9
1957.3636 z=9
1961.1357 z=9
1968.5770 z=9
1972.1328 z=9
1953.2299 z=9
1907.6716 z=?
2515.6057 z=7
2514.7441 z=7
2520.8860 z=7
2529.5974 z=7
2426.2876 z=7
2426.7205 z=7
2427.7249 z=7
2428.2969 z=7


20230308_20230227_Mb10uM+100mMK3PO4+Ar+RT2H_z8_2201_Sample_1_1 #20 RT: 0.24 AV: 1 NL: 1.07E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2201.3999@cid1.00 [200.0000-3500.0000]
Myoglobin_Sample
MS/MS_1
Relative Abundance
m/z
2201.2791 z=8
616.1695 z=1
617.1733 z=1
2427.7209 z=7
2427.8645 z=7
2195.7786 z=8
1916.5001 z=2
209.2594 z=?
1050.5129 z=1
967.4401 z=1
1721.2229 z=3
2124.1311 z=8
2421.2910 z=7
2489.3120 z=5
521.2658 z=1
571.1724 z=1
619.1814 z=1
806.3946 z=1
1213.6077 z=3
1309.3519 z=3
1591.1614 z=3
1814.9565 z=2
1963.0214 z=2
2665.0479 z=5
2788.4807 z=5
2994.5684 z=2
3259.5081 z=4
3371.7229 z=?


20230308_20230227_Mb10uM+100mMK3PO4+Ar+RT2H_z8_2201_Sample_1_2 #20 RT: 0.24 AV: 1 NL: 1.06E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2201.3999@cid1.00 [200.0000-3500.0000]
Myoglobin_Sample
MS/MS_2
2201.2795 z=8
616.1696 z=1
617.1734 z=1
204.0957 z=?
521.2659 z=1
571.1725 z=1
619.1814 z=1
806.3948 z=1
967.4404 z=1
1050.5132 z=1
1213.6078 z=3
1309.3523 z=3
1591.1617 z=3
1721.2233 z=3
1814.9569 z=2
1916.5007 z=2
1963.0219 z=2
2124.1316 z=8
2195.7791 z=8
2421.2915 z=7
2427.7214 z=7
2427.8650 z=7
2541.8599 z=6
2665.0486 z=5
2607.4006 z=5
3054.6465 z=4
3258.7568 z=4
Relative Abundance
m/z


20230308_20230227_Mb10uM+100mMK3PO4+Ar+RT2H_z8_2201_Sample_1_3 #20 RT: 0.24 AV: 1 NL: 1.06E6
T: FTMS + p NSI sid=15.00 cv=15.00 Full ms2 2201.3999@cid1.00 [200.0000-3500.0000]
Myoglobin_Sample
MS/MS_3
Relative Abundance
m/z
2201.2795 z=8
616.1696 z=1
617.1734 z=1
204.0957 z=?
521.2659 z=1
571.1725 z=1
619.1814 z=1
806.3948 z=1
967.4404 z=1
1050.5132 z=1
1213.6078 z=3
1309.3523 z=3
1591.1617 z=3
1721.5581 z=3
1814.9569 z=2
1916.5006 z=2
1963.0217 z=2
2124.1316 z=8
2195.7791 z=8
2421.2913 z=7
2427.7214 z=7
2427.8647 z=7
2489.3123 z=5
2665.0486 z=5
2607.4006 z=5
3054.6465 z=4
3259.5085 z=4