Fig. S1-A

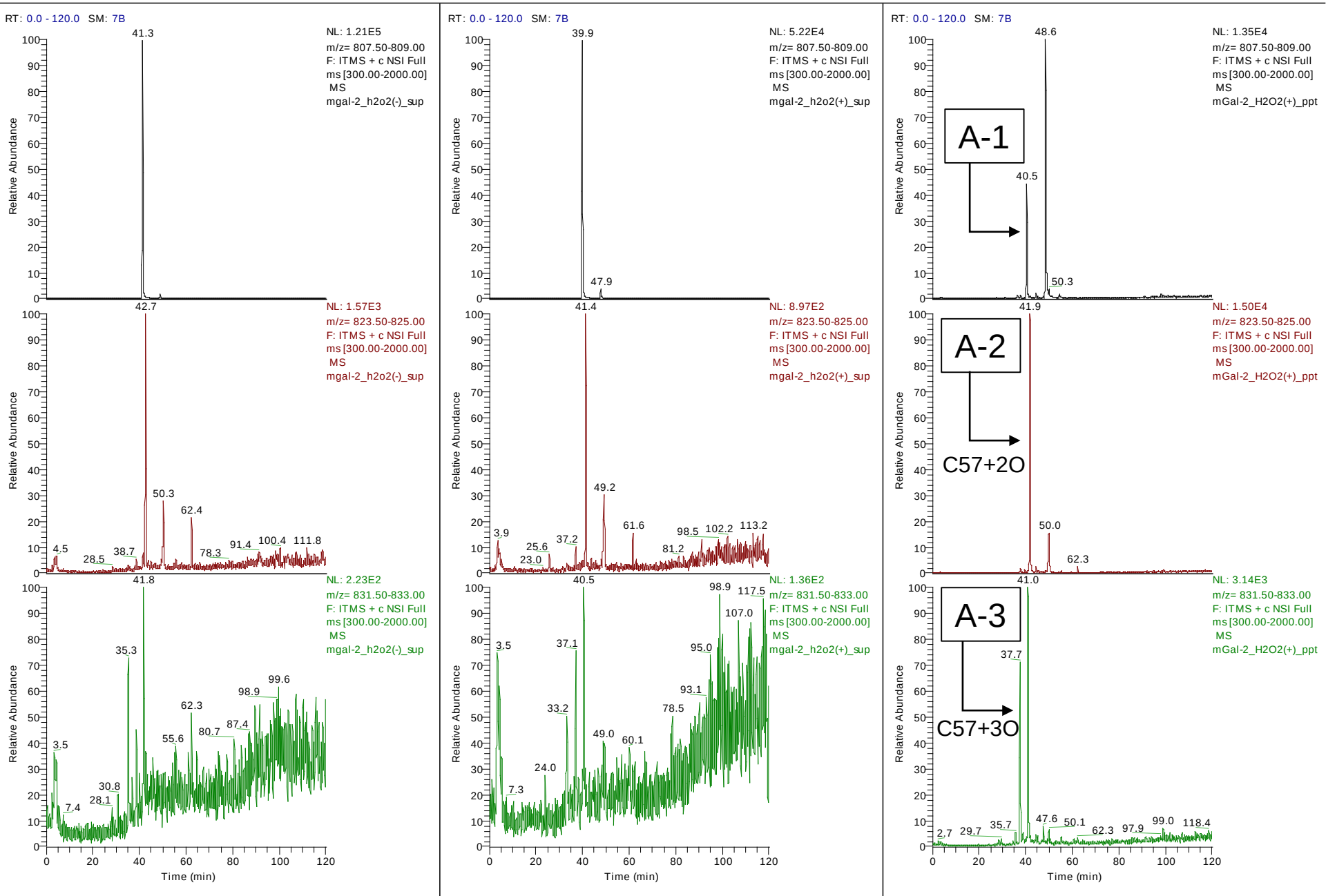

RT: 0.0 - 120.0 SM: 7B
NL: 1.21E5
m/z= 807.50-809.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 1.57E3
m/z= 823.50-825.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 2.23E2
m/z= 831.50-833.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 5.22E4
m/z= 807.50-809.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 8.97E2
m/z= 823.50-825.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 1.36E2
m/z= 831.50-833.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 1.35E4
m/z= 807.50-809.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
NL: 1.50E4
m/z= 823.50-825.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
NL: 3.14E3
m/z= 831.50-833.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
A-1
A-2
C57+2O
A-3
C57+3O
Relative Abundance
Time (min)

Fig. S1-A. Full region of the mass chromatograms shown in Fig. 1A. Left, middle, and right columns correspond to supernatant of non-oxidized sample, supernatant of oxidized sample, and precipitate of oxidized sample, respectively. Upper, middle, and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=807.85, mass range: m/z 807.5-809), theoretical molecular weight plus 32 ($[M+2O+2H]^{2+}$=823.85, mass range: m/z 823.5-825), and theoretical molecular weight plus 48 ($[M+3O+2H]^{2+}$=831.85, mass range: m/z 831.5-833), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.

Fig. S1-A (A-1, A-2, A-3) (a)

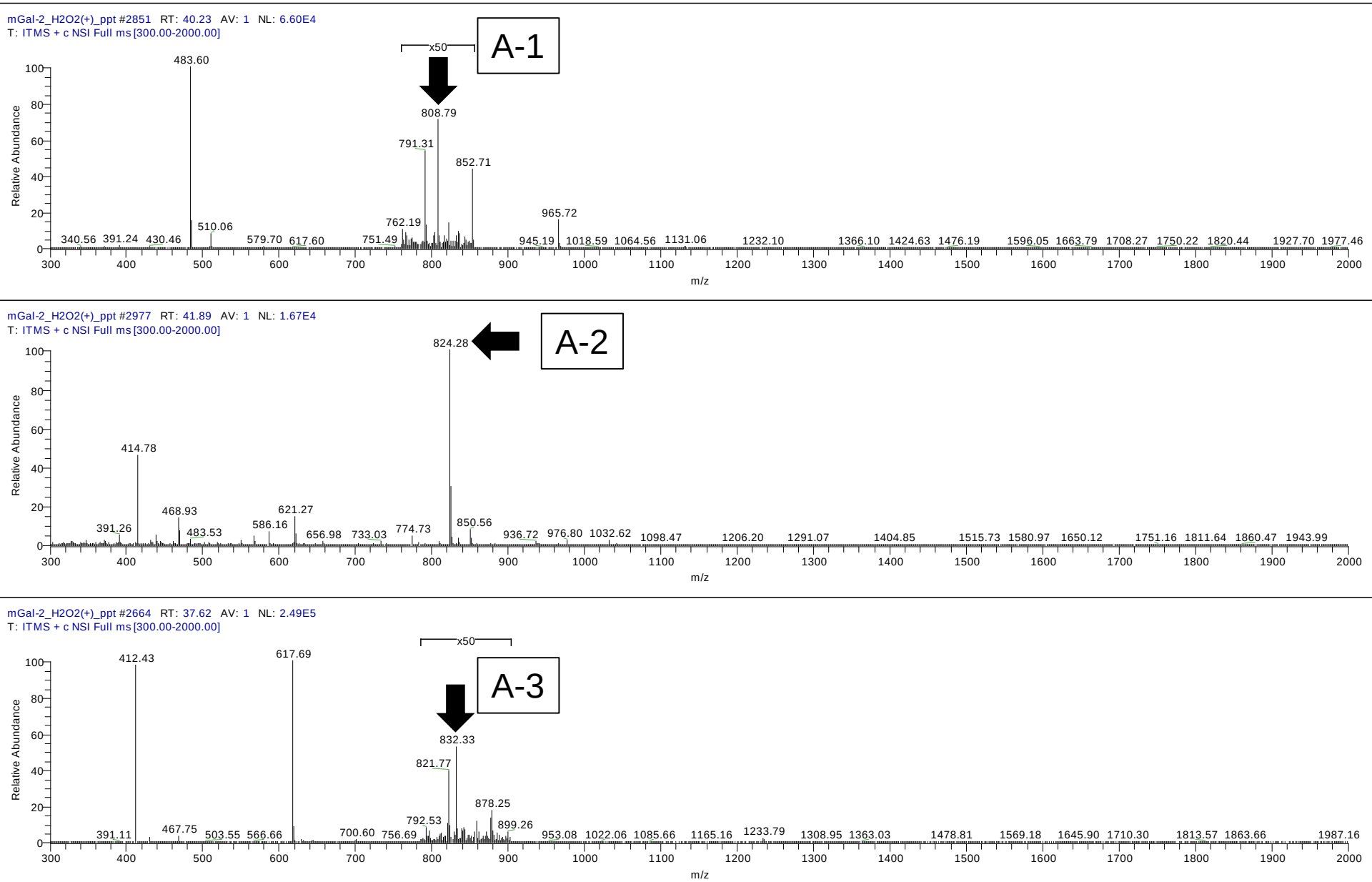
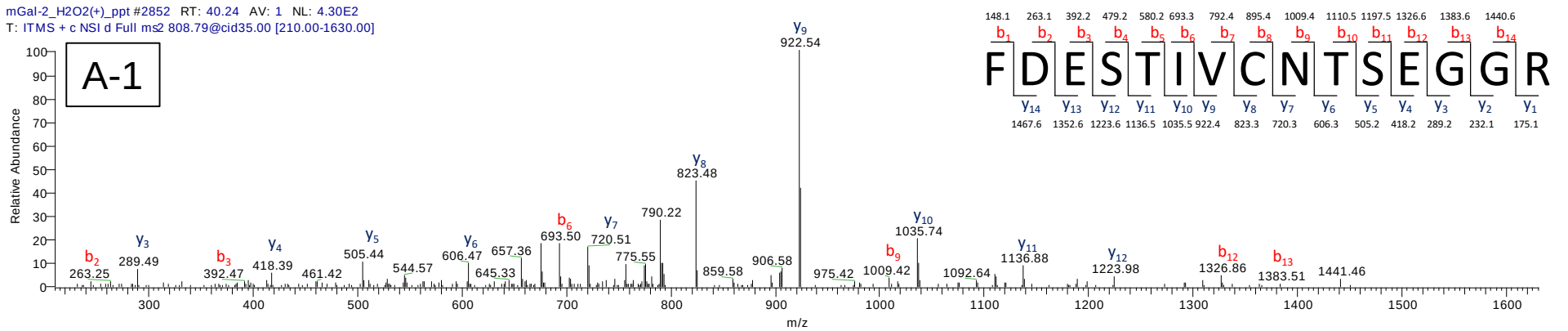
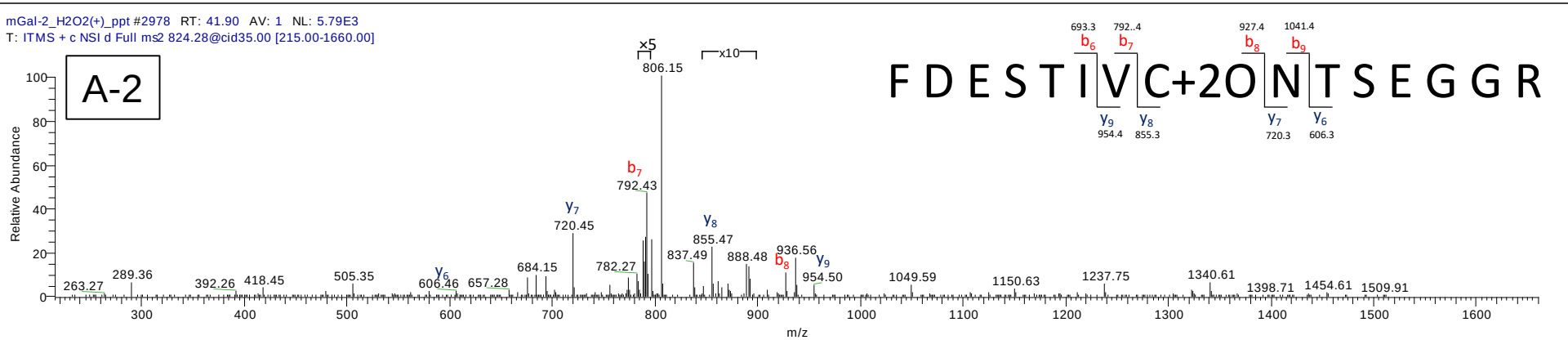


Fig. S1-A (A-1, A-2, A-3) (a). MS spectra of the LC fractions containing the ions A-1, A-2, A-3 shown in Fig. S1-A. Arrowheads indicate the peaks for peptides subjected to MS/MS analyses shown in Fig. S1-A (A-1, A-2, A-3) (b).

Fig. S1-A (A-1, A-2, A-3) (b)





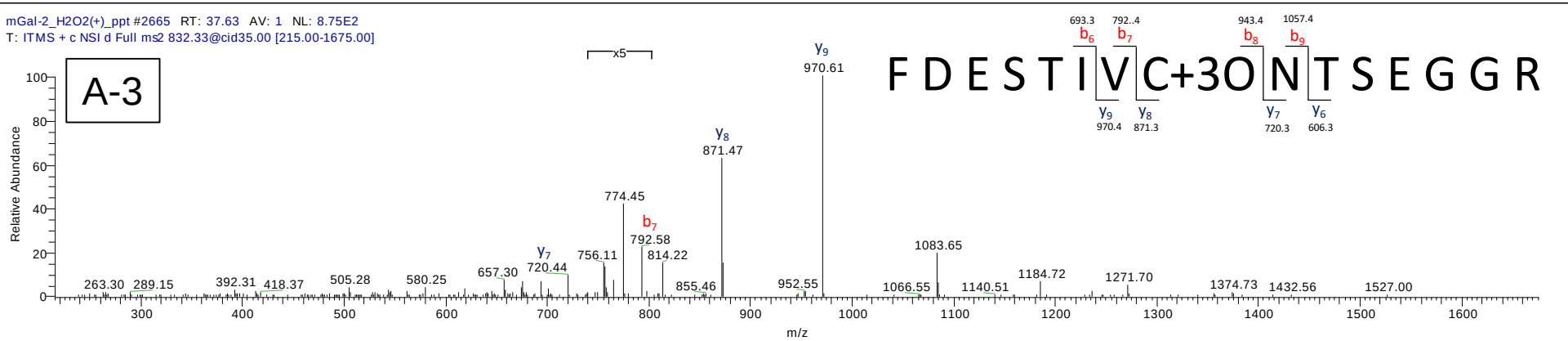
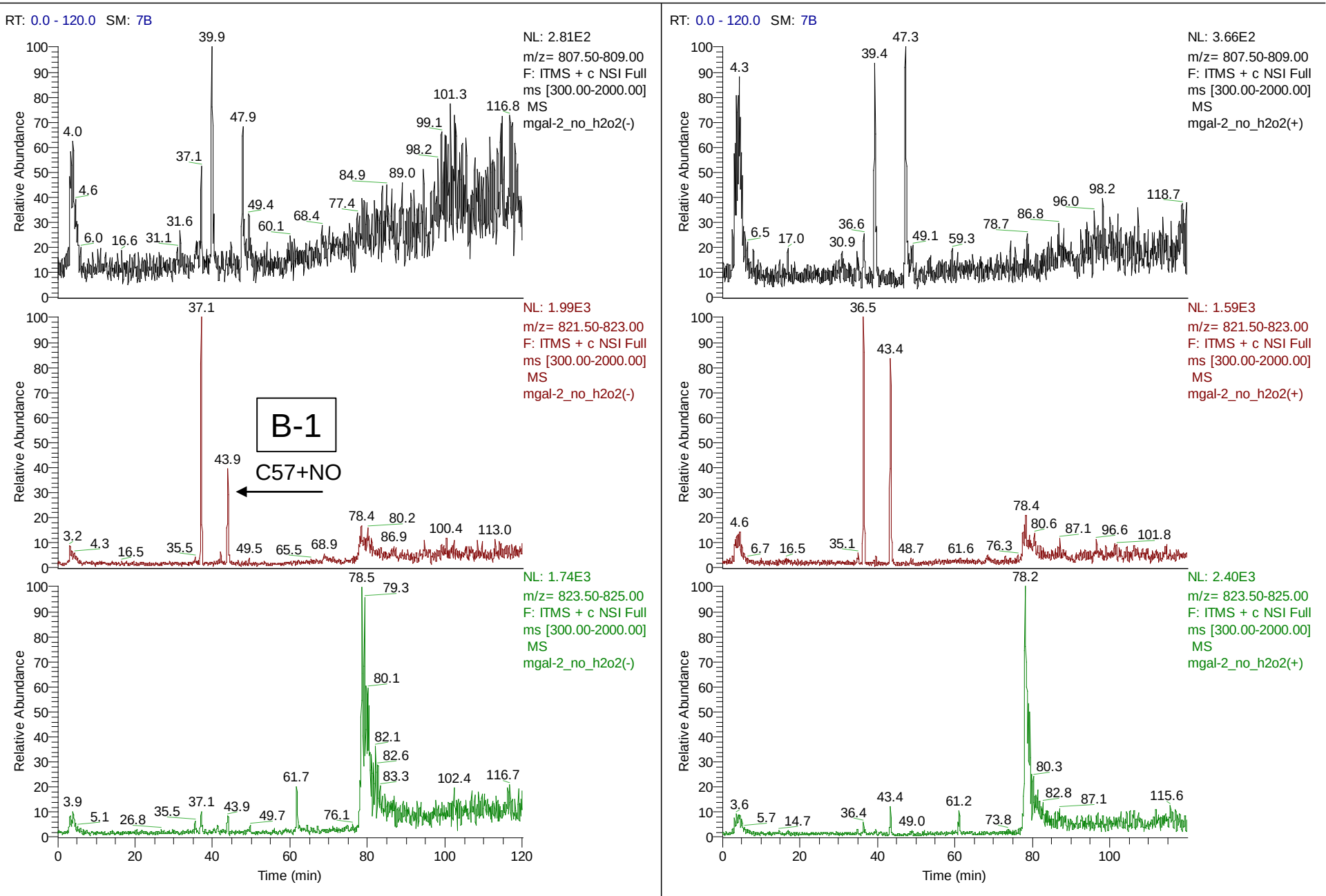


Fig. S1-A (A-1, A-2, A-3) (b). MS/MS spectra of the ions A-1, A-2, and A-3 shown in Fig. S1-A.

Fig. S1-B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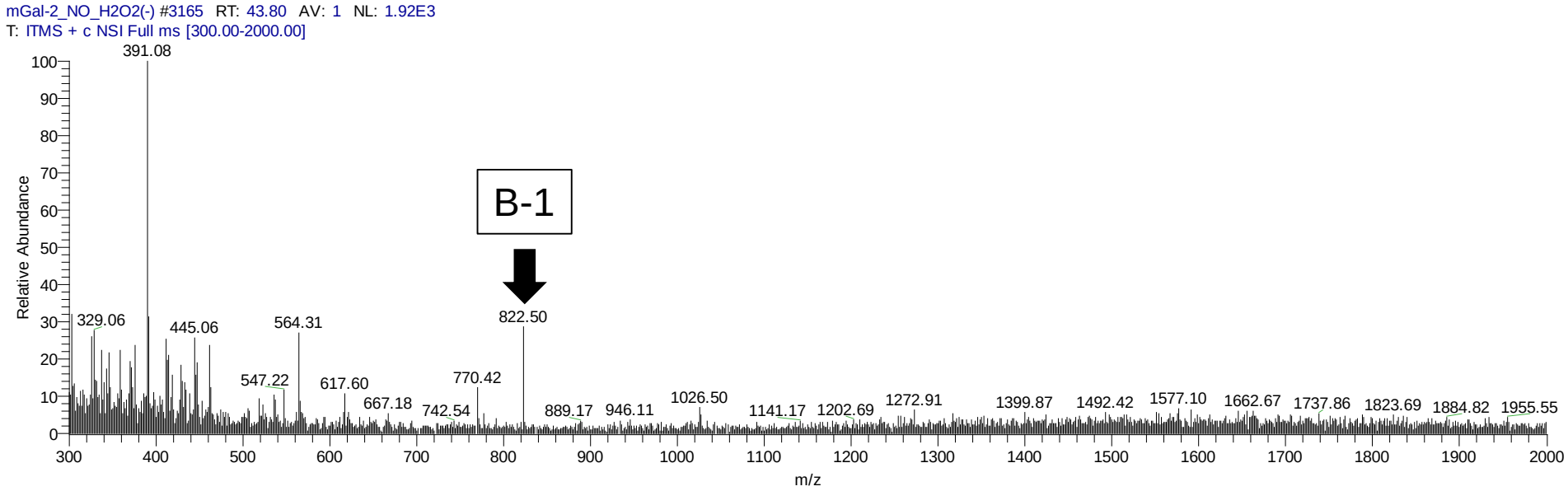
NL: 2.81E2
m/z= 807.50-809.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 3.66E2
m/z= 807.50-809.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
NL: 1.99E3
m/z= 821.50-823.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 1.59E3
m/z= 821.50-823.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
NL: 1.74E3
m/z= 823.50-825.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 2.40E3
m/z= 823.50-825.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
B-1
C57+NO
Relative Abundance
Time (min)

Fig. S1-B. Full region of the mass chromatograms shown in Fig. 1B. Left and right columns correspond to supernatant of non-oxidized sample and oxidized sample, respectively. Upper, middle, and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=807.85, mass range: m/z 807.5-809), theoretical molecular weight plus 29 ($[M+NO+H]^{2+}$=822.35, mass range: m/z 821.5-823), and theoretical molecular weight plus 32 ($[M+2O+2H]^{2+}$=823.85, mass range: m/z 823.5-825), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.

Fig. S1-B (B-1)


mGal-2_NO_H2O2(-) #3165 RT: 43.80 AV: 1 NL: 1.92E3
T: ITMS + c NSI Full ms [300.00-2000.00]
B-1
Relative Abundance
m/z
391.08
329.06
445.06
564.31
547.22
617.60
667.18
742.54
770.42
822.50
889.17
946.11
1026.50
1141.17
1202.69
1272.91
1399.87
1492.42
1577.10
1662.67
1737.86
1823.69
1884.82
1955.55

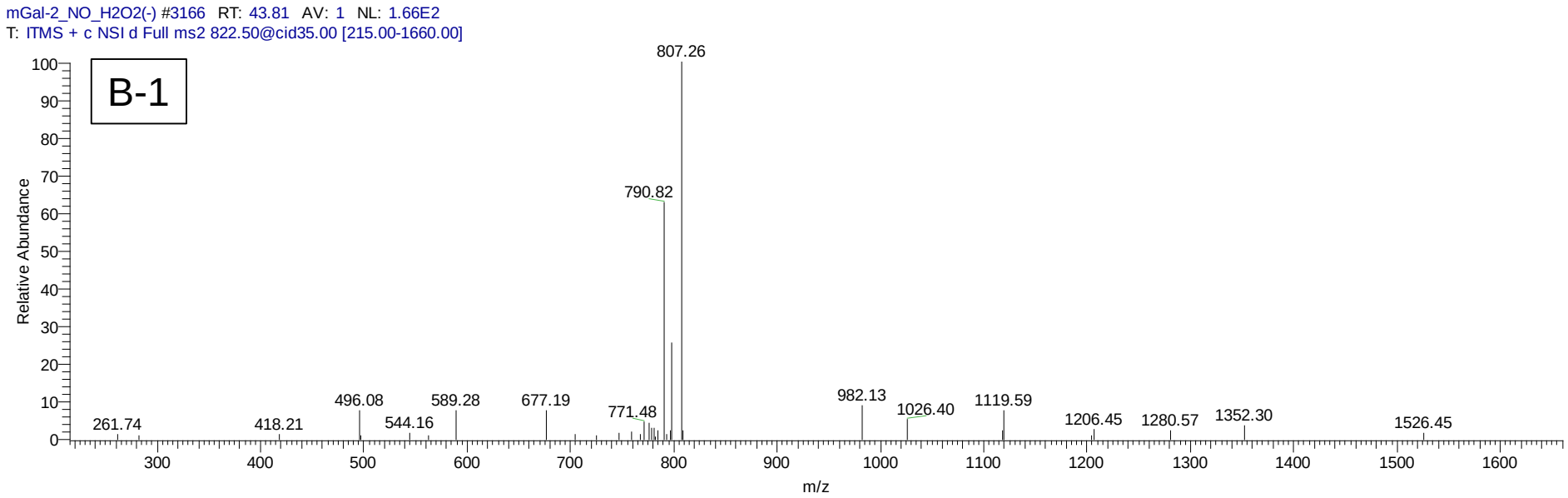

mGal-2_NO_H2O2(-) #3166 RT: 43.81 AV: 1 NL: 1.66E2
T: ITMS + c NSI d Full ms2 822.50@cid35.00 [215.00-1660.00]
B-1
Relative Abundance
m/z
807.26
790.82
261.74
418.21
496.08
544.16
589.28
677.19
771.48
982.13
1026.40
1119.59
1206.45
1280.57
1352.30
1526.45

Fig. S1-B (B-1). (Top) MS spectrum of the LC fraction containing the ion B-1 shown in Fig. S1-B. Arrowhead indicates the peak for the peptide subjected to MS/MS analysis. (Bottom) MS/MS spectrum of the ion B-1 shown in Fig. S1-B.

Fig. S1-C

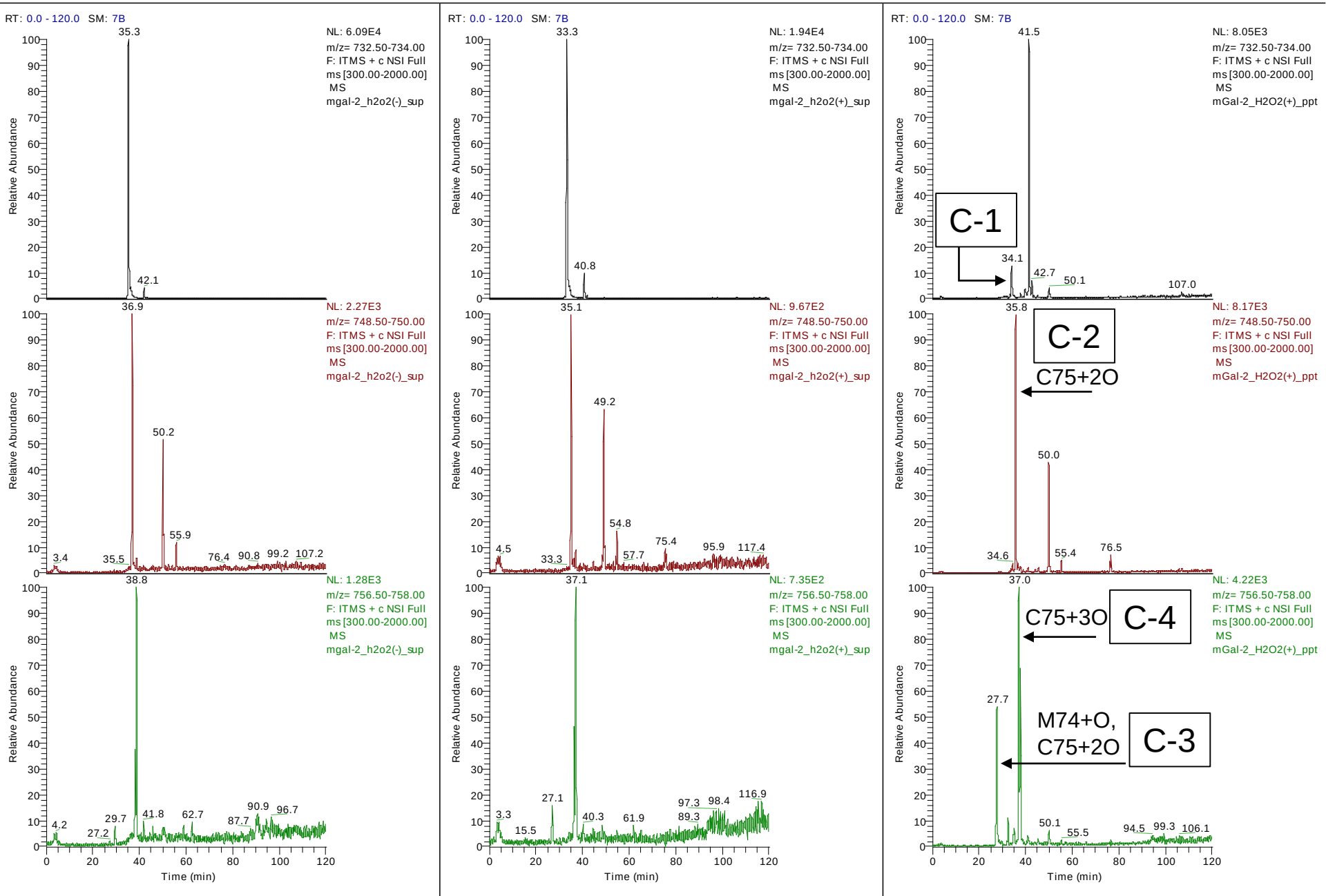
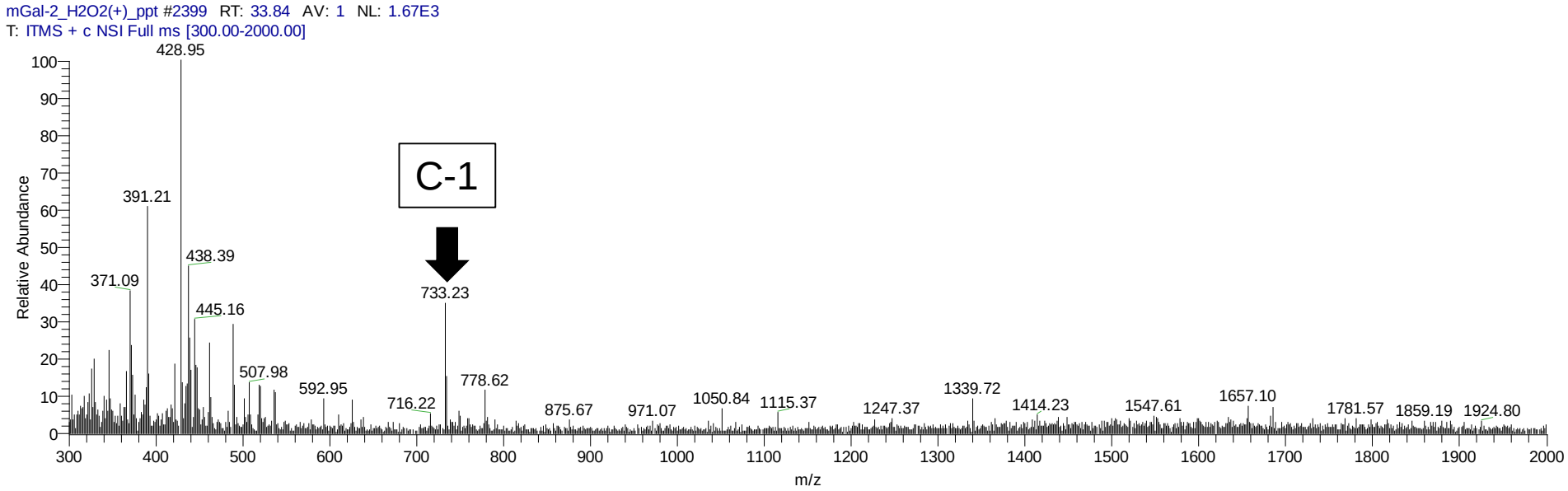

RT: 0.0 - 120.0 SM: 7B
NL: 6.09E4
m/z= 732.50-734.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 2.27E3
m/z= 748.50-750.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 1.28E3
m/z= 756.50-758.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
NL: 1.94E4
m/z= 732.50-734.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 9.67E2
m/z= 748.50-750.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 7.35E2
m/z= 756.50-758.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
NL: 8.05E3
m/z= 732.50-734.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
NL: 8.17E3
m/z= 748.50-750.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
NL: 4.22E3
m/z= 756.50-758.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
C-1
C-2
C75+2O
C75+3O
C-4
M74+O,
C75+2O
C-3
Relative Abundance
Time (min)

Fig. S1-C. Full region of the mass chromatograms shown in Fig. 1C. Left, middle, and right columns correspond to supernatant of non-oxidized sample, supernatant of oxidized sample, and precipitate of oxidized sample, respectively. Upper, middle, and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=732.82, mass range: m/z 732.5-734), theoretical molecular weight plus 32 ($[M+2O+2H]^{2+}$=748.81, mass range: m/z 748.5-750), and theoretical molecular weight plus 48 ($[M+3O+2H]^{2+}$=756.82, mass range: m/z 756.5-758), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.

Fig. S1-C (C-1, C-2) (a)



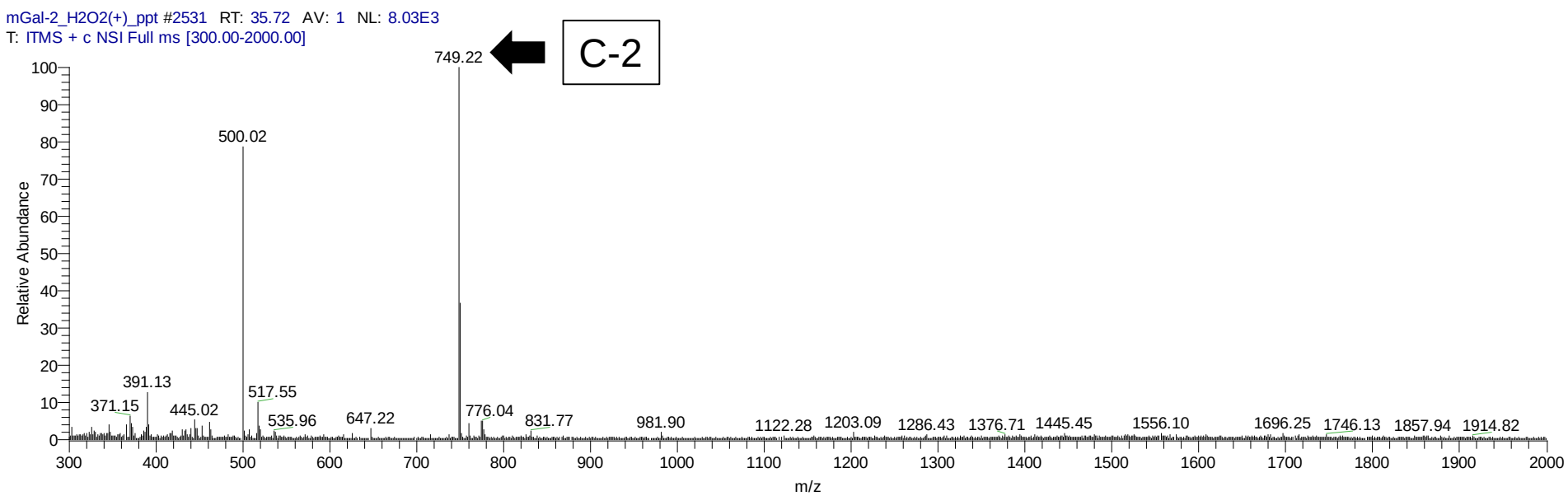
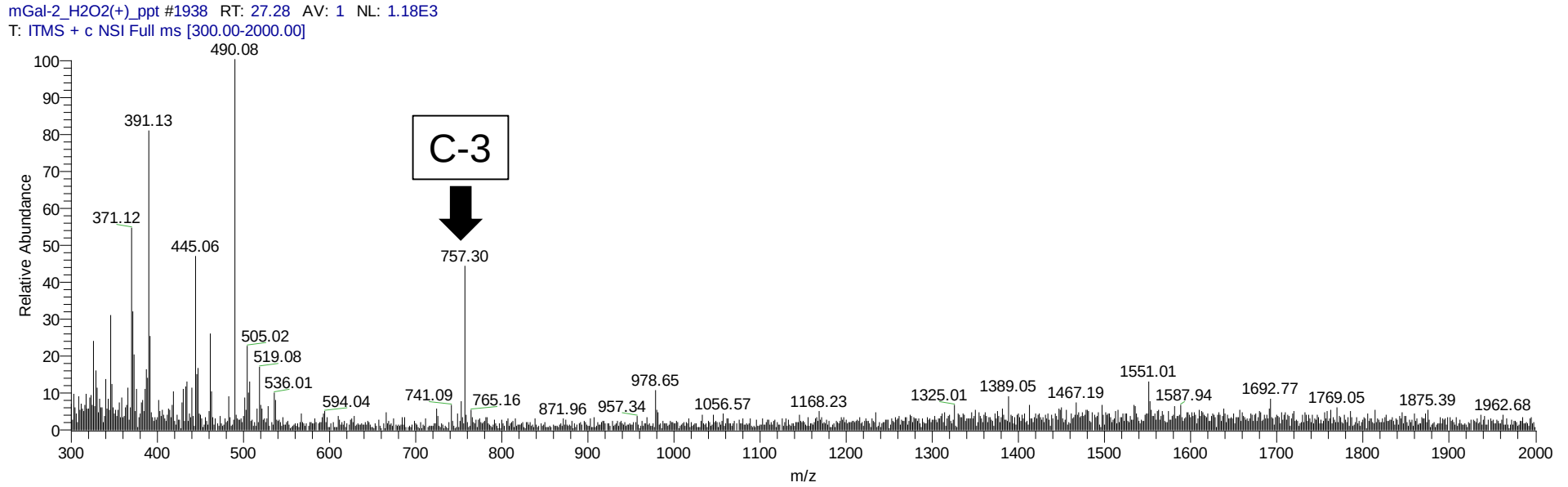


Fig. S1-C (C-1, C-2) (a). MS spectra of the LC fractions containing the ions C-1 and C-2 shown in Fig. S1-C. Arrowheads indicate the peaks for peptides subjected to MS/MS analyses shown in Fig. S1-C (C-1, C-2) (b).

Fig. S1-C (C-3, C-4) (a)



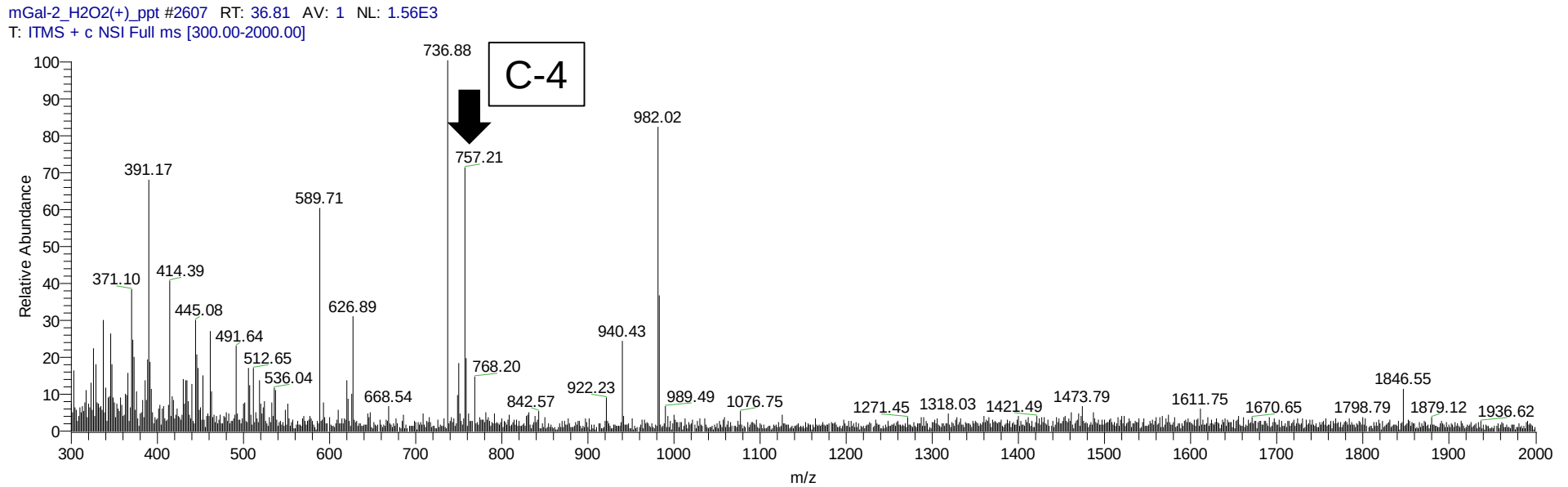
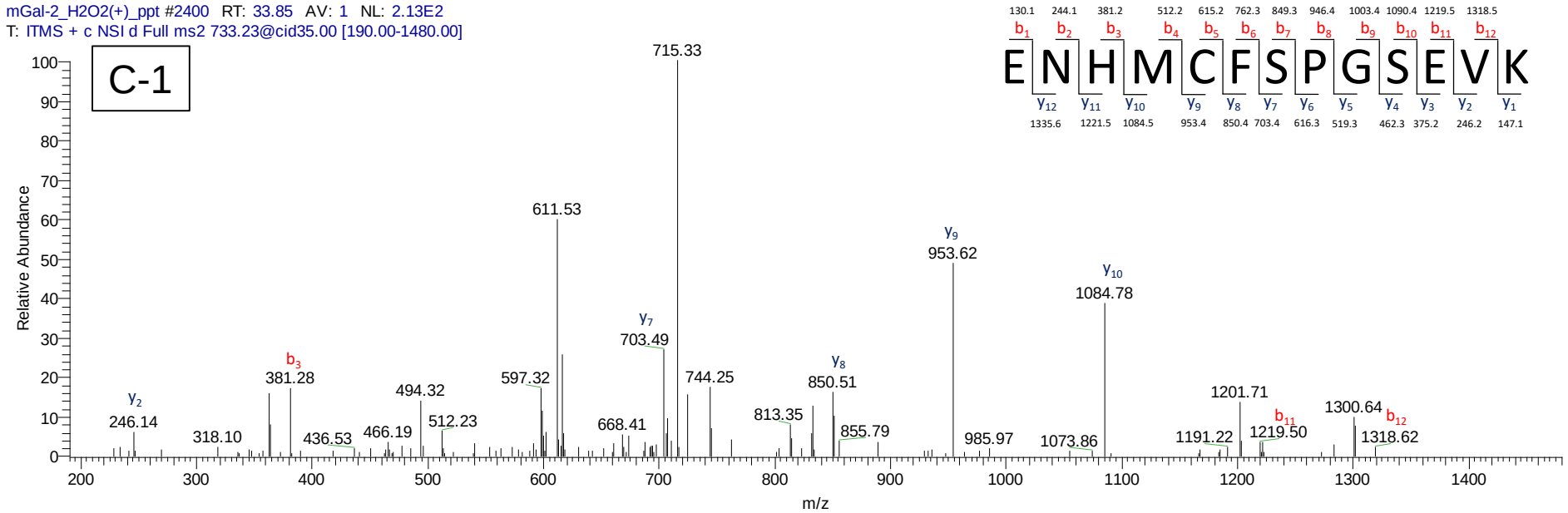


Fig. S1-C (C-3, C-4) (a). MS spectra of the LC fractions containing the ions C-3 and C-4 shown in Fig. S1-C. Arrowheads indicate the peaks for peptides subjected to MS/MS analyses shown in Fig. S1-C (C-3, C-4) (b).

Fig. S1-C (C-1, C-2) (b)



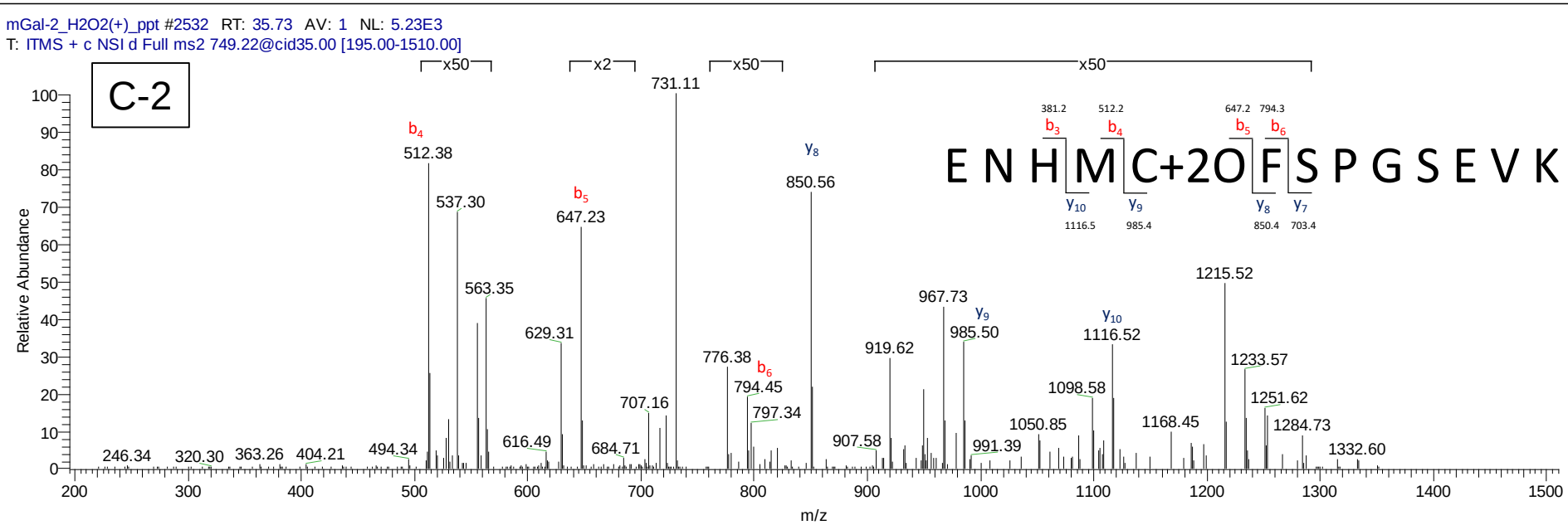
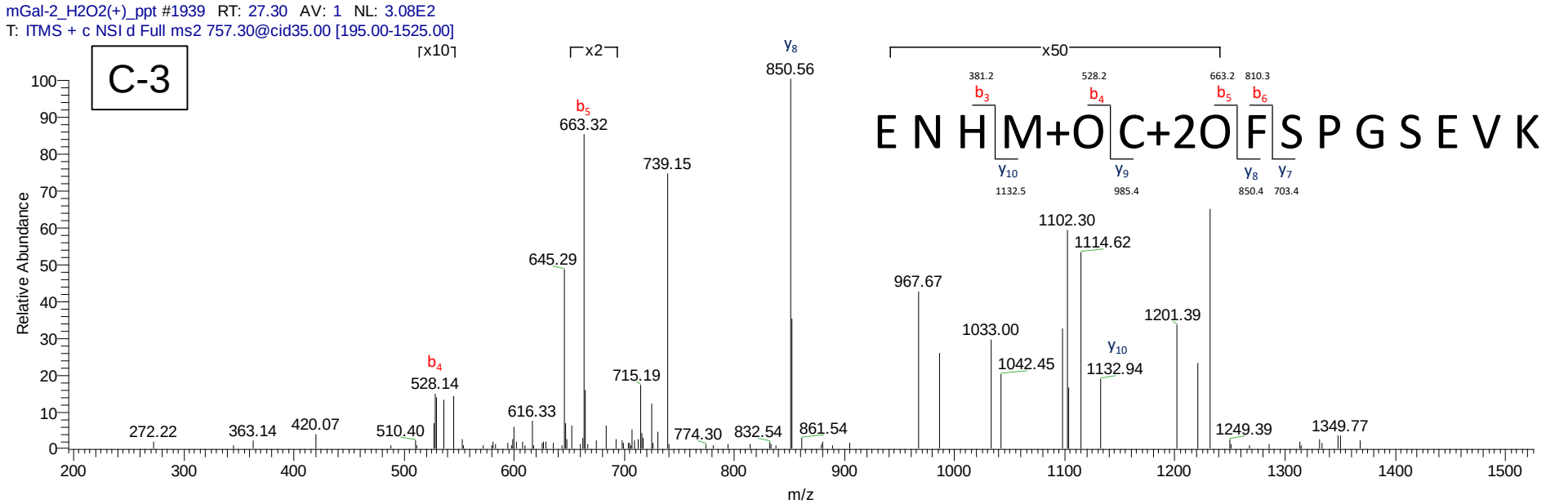


Fig. S1-C (C-1, C-2) (b). MS/MS spectra of the ions C-1 and C-2 shown in Fig. S1-C.

Fig. S1-C (C-3, C-4) (b)



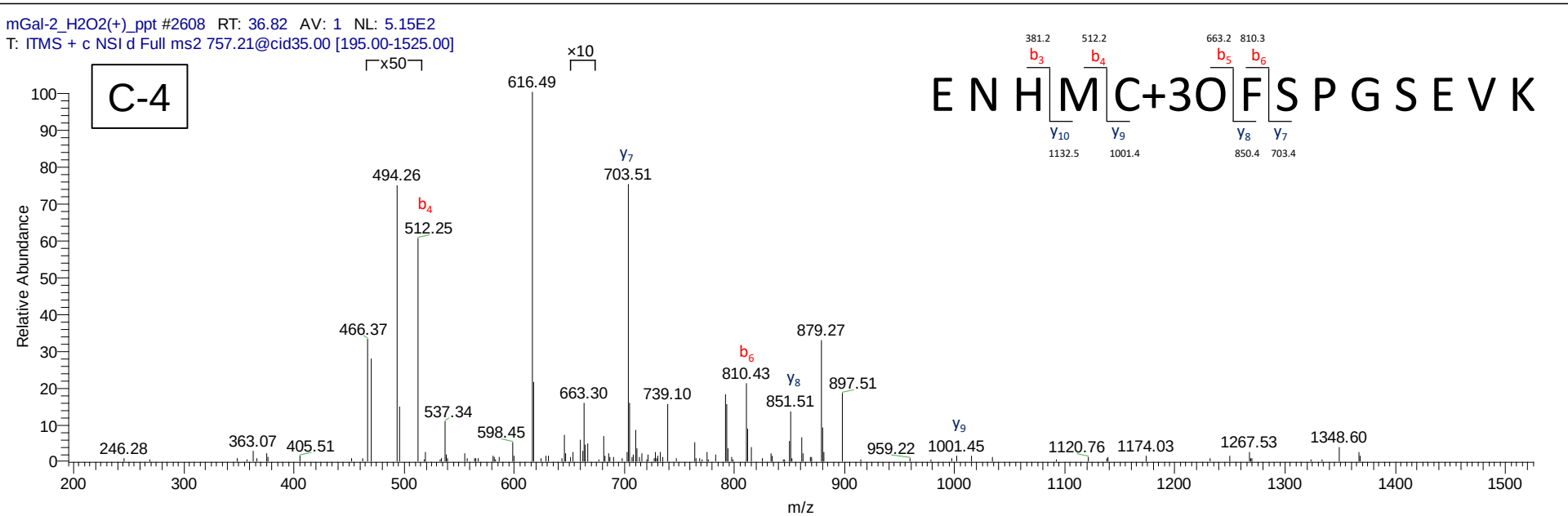


Fig. S1-C (C-3, C-4) (b). MS/MS spectra of the ions C-3 and C-4 shown in Fig. S1-C.

Fig. S1-D

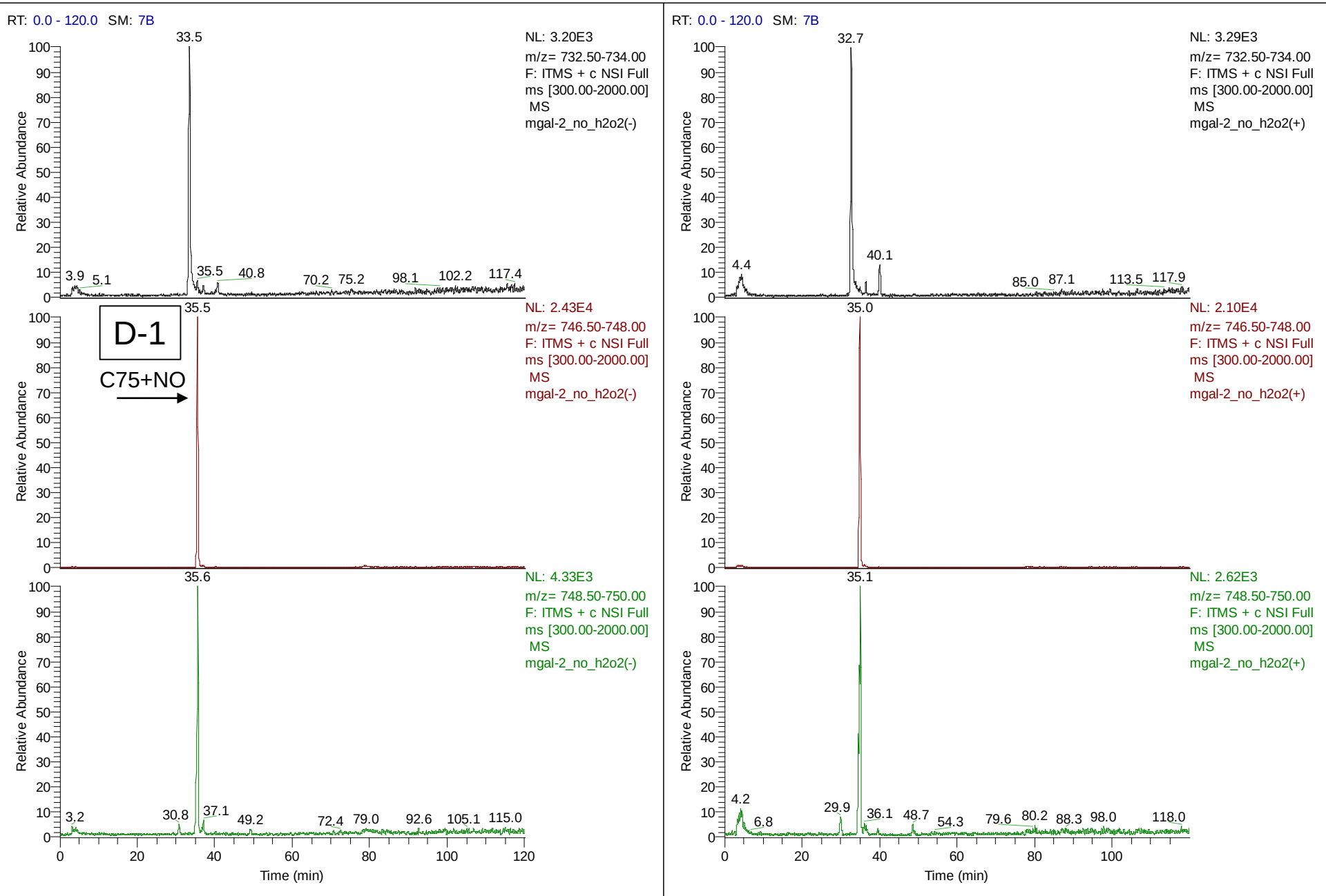
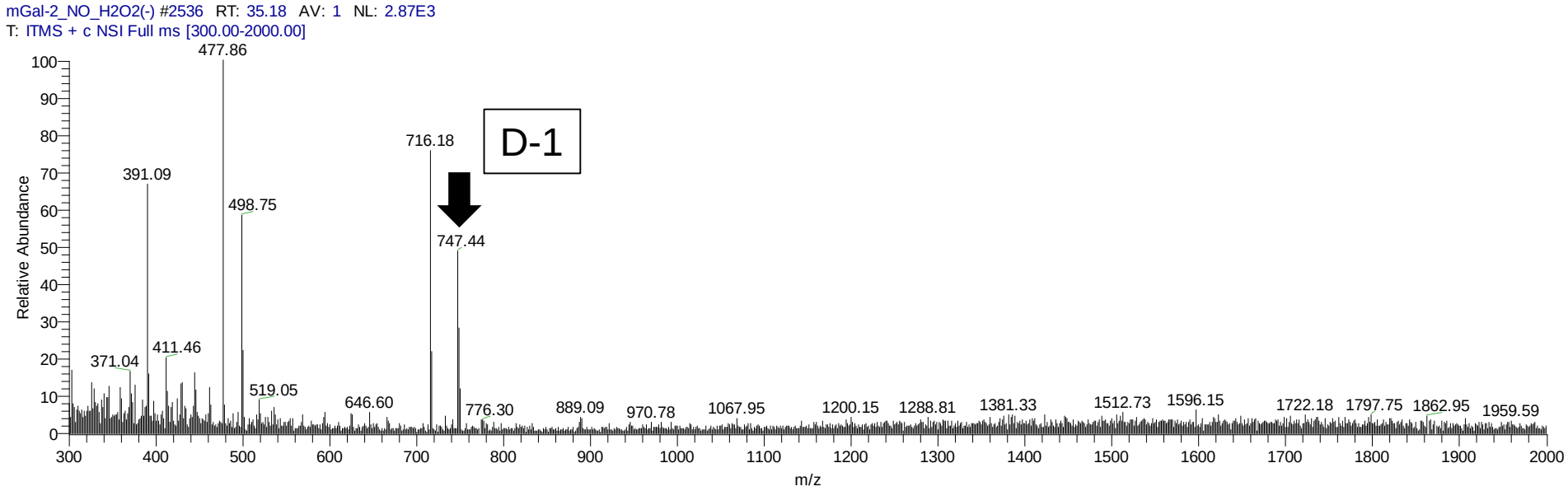

RT: 0.0 - 120.0 SM: 7B
NL: 3.20E3
m/z= 732.50-734.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 3.29E3
m/z= 732.50-734.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
D-1
C75+NO
NL: 2.43E4
m/z= 746.50-748.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 2.10E4
m/z= 746.50-748.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
NL: 4.33E3
m/z= 748.50-750.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
NL: 2.62E3
m/z= 748.50-750.00
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
Relative Abundance
Time (min)

Fig. S1-D. Full region of the mass chromatograms shown in Fig. 1D. Left and right columns correspond to supernatant of non-oxidized sample and oxidized sample, respectively. Upper, middle, and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=732.82, mass range: m/z 732.5-734), theoretical molecular weight plus 29 ($[M+NO+H]^{2+}$=747.31, mass range: m/z 746.5-748), and theoretical molecular weight plus 32 ($[M+2O+2H]^{2+}$=748.81, mass range: m/z 748.5-750), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.

Fig. S1-D (D-1)


mGal-2_NO_H2O2(-) #2536 RT: 35.18 AV: 1 NL: 2.87E3
T: ITMS + c NSI Full ms [300.00-2000.00]
D-1
Relative Abundance
m/z
477.86
716.18
391.09
498.75
747.44
411.46
371.04
519.05
646.60
776.30
889.09
970.78
1067.95
1200.15
1288.81
1381.33
1512.73
1596.15
1722.18
1797.75
1862.95
1959.59

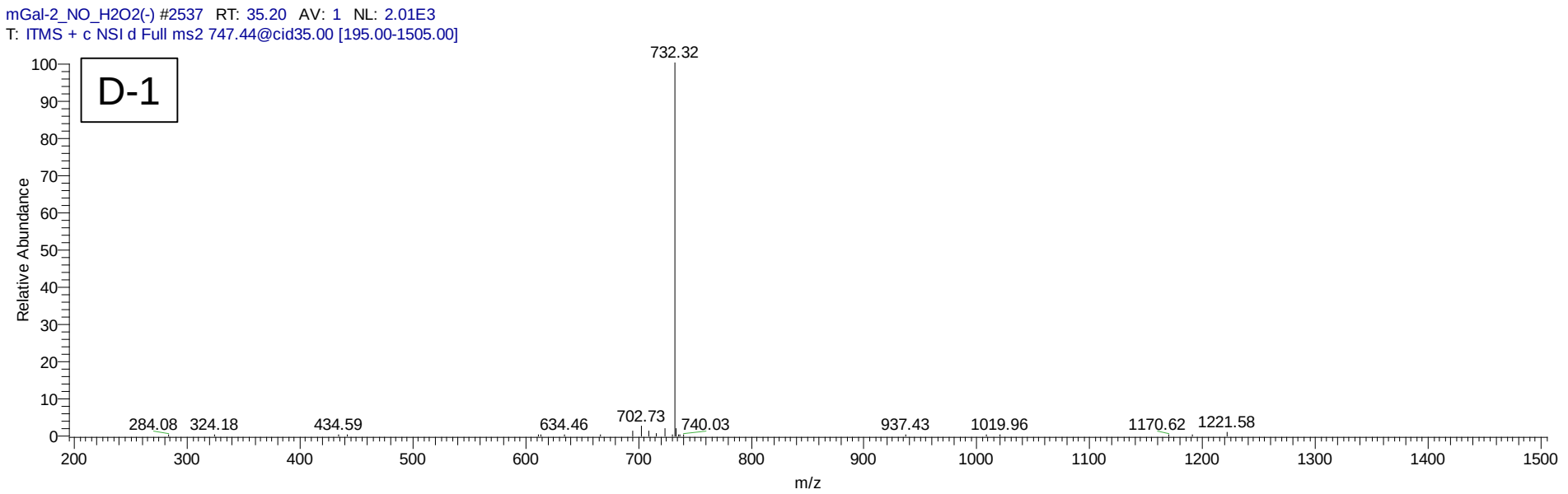

mGal-2_NO_H2O2(-) #2537 RT: 35.20 AV: 1 NL: 2.01E3
T: ITMS + c NSI d Full ms2 747.44@cid35.00 [195.00-1505.00]
D-1
Relative Abundance
m/z
732.32
284.08
324.18
434.59
634.46
702.73
740.03
937.43
1019.96
1170.62
1221.58

Fig. S1-D (D-1). (Top) MS spectrum of the LC fraction containing the ion D-1 shown in Fig. S1-D. Arrowhead indicates the peak for the peptide subjected to MS/MS analysis. (Bottom) MS/MS spectrum of the ion D-1 shown in Fig. S1-D.

Fig. S1-E

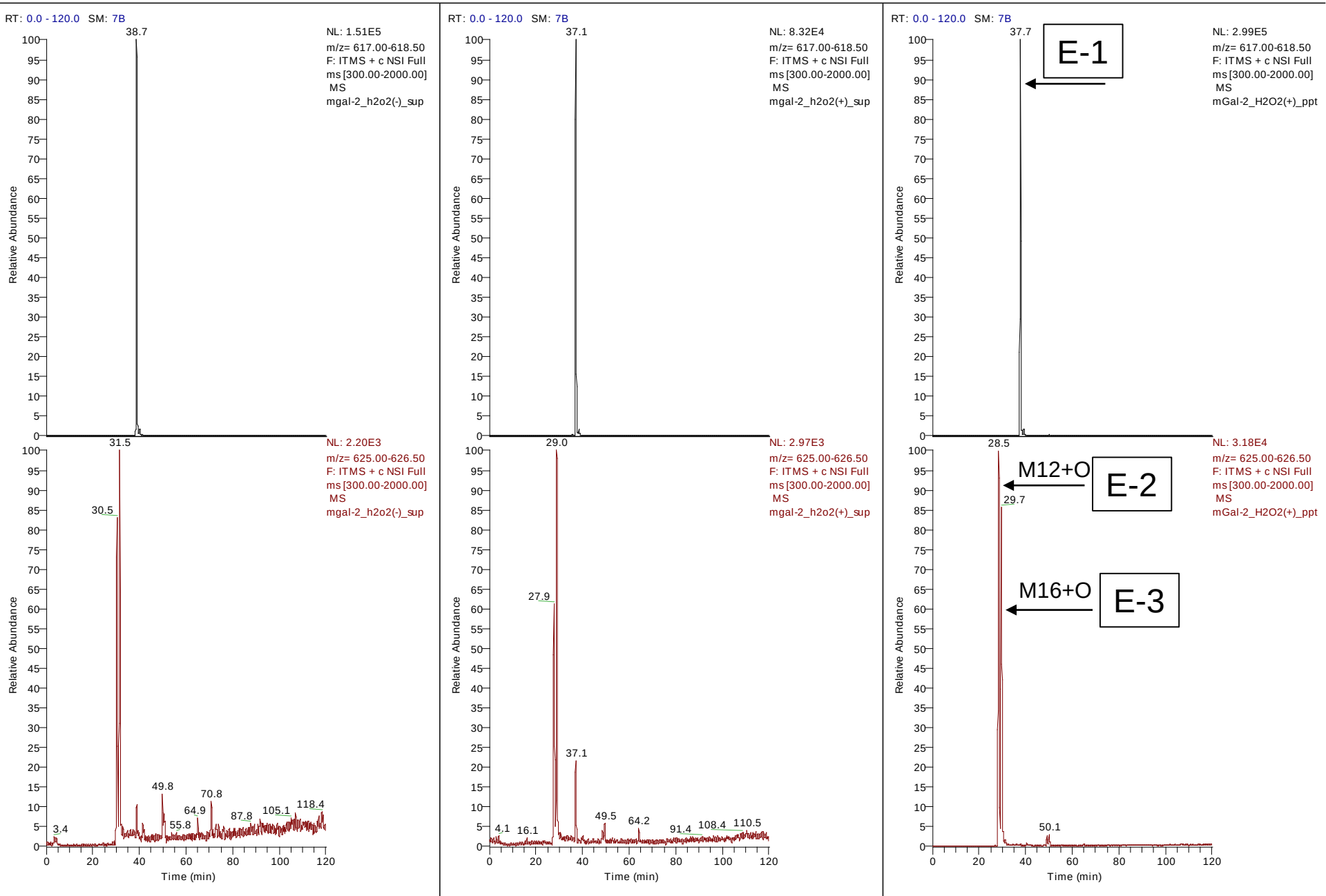
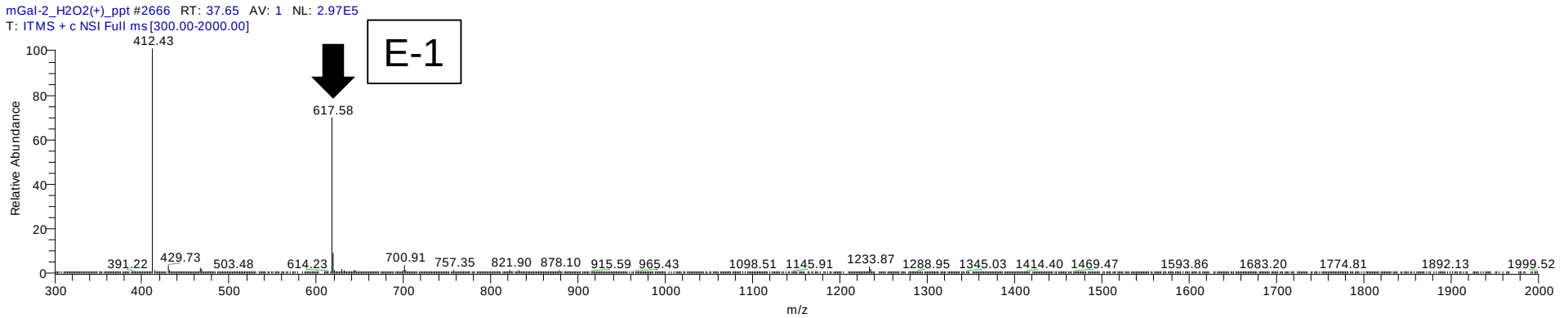
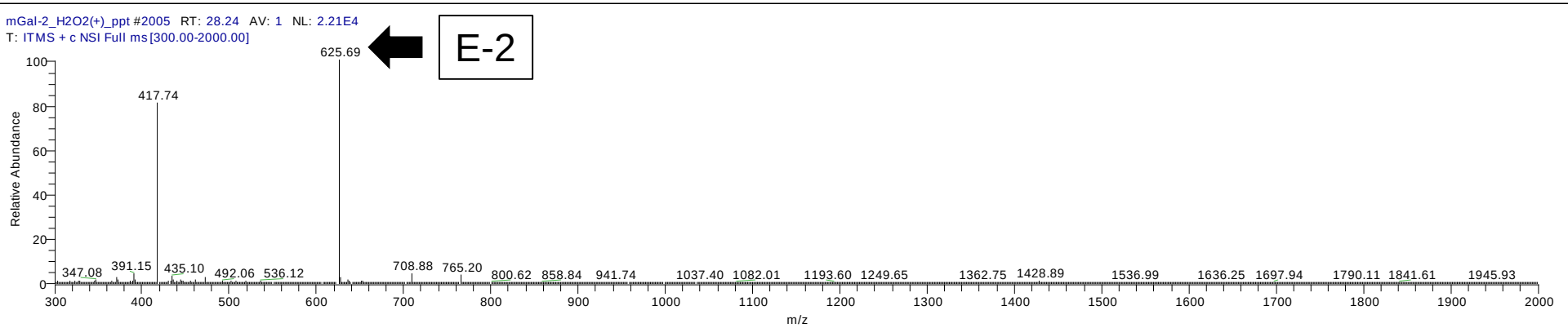

RT: 0.0 - 120.0 SM: 7B
38.7
NL: 1.51E5
m/z= 617.00-618.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
31.5
NL: 2.20E3
m/z= 625.00-626.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(-)_sup
30.5
3.4
49.8
55.8
64.9
70.8
87.8
105.1
118.4
37.1
NL: 8.32E4
m/z= 617.00-618.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
29.0
NL: 2.97E3
m/z= 625.00-626.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_h2o2(+)_sup
27.9
37.1
4.1
16.1
49.5
64.2
91.4
108.4
110.5
37.7
E-1
NL: 2.99E5
m/z= 617.00-618.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
28.5
M12+O
E-2
29.7
NL: 3.18E4
m/z= 625.00-626.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mGal-2_H2O2(+)_ppt
M16+O
E-3
50.1
Relative Abundance
Time (min)

Fig. S1-E. Full region of the mass chromatograms shown in Fig. 1E. Left, middle, and right columns correspond to supernatant of non-oxidized sample, supernatant of oxidized sample, and precipitate of oxidized sample, respectively. Upper and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=617.32, mass range: m/z 617-618.5) and theoretical molecular weight plus 16 ($[M+O+2H]^{2+}$=625.32, mass range: m/z 625-626.5), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.

Fig. S1-E (E-1, E-2, E-3) (a)





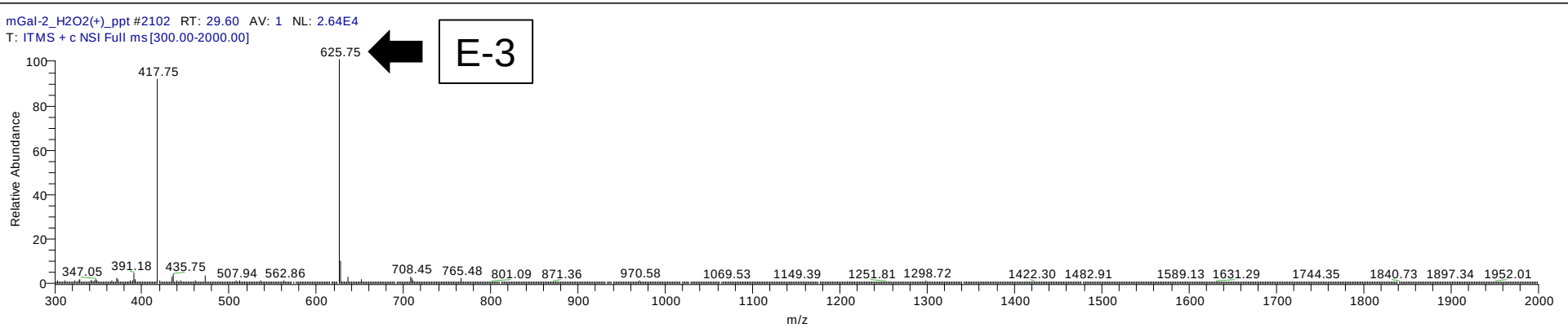


Fig. S1-E (E-1, E-2, E-3) (a). MS spectra of the LC fractions containing the ions E-1, E-2, and E-3 shown in Fig. S1-E. Arrowheads indicate the peaks for peptides subjected to MS/MS analyses shown in Fig. S1-E (E-1, E-2, E-3) (b).

Fig. S1-E (E-1, E-2, E-3) (b)

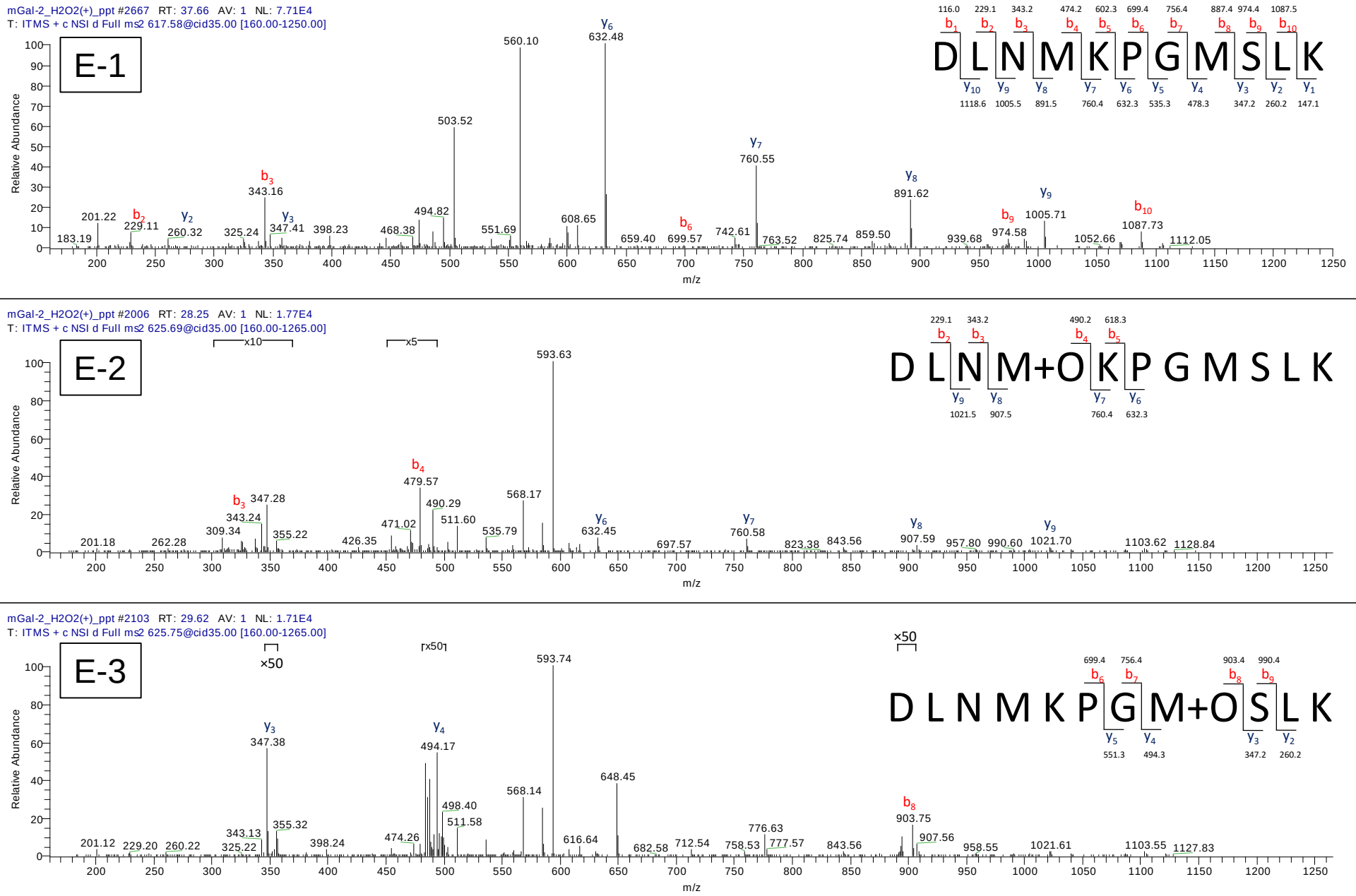
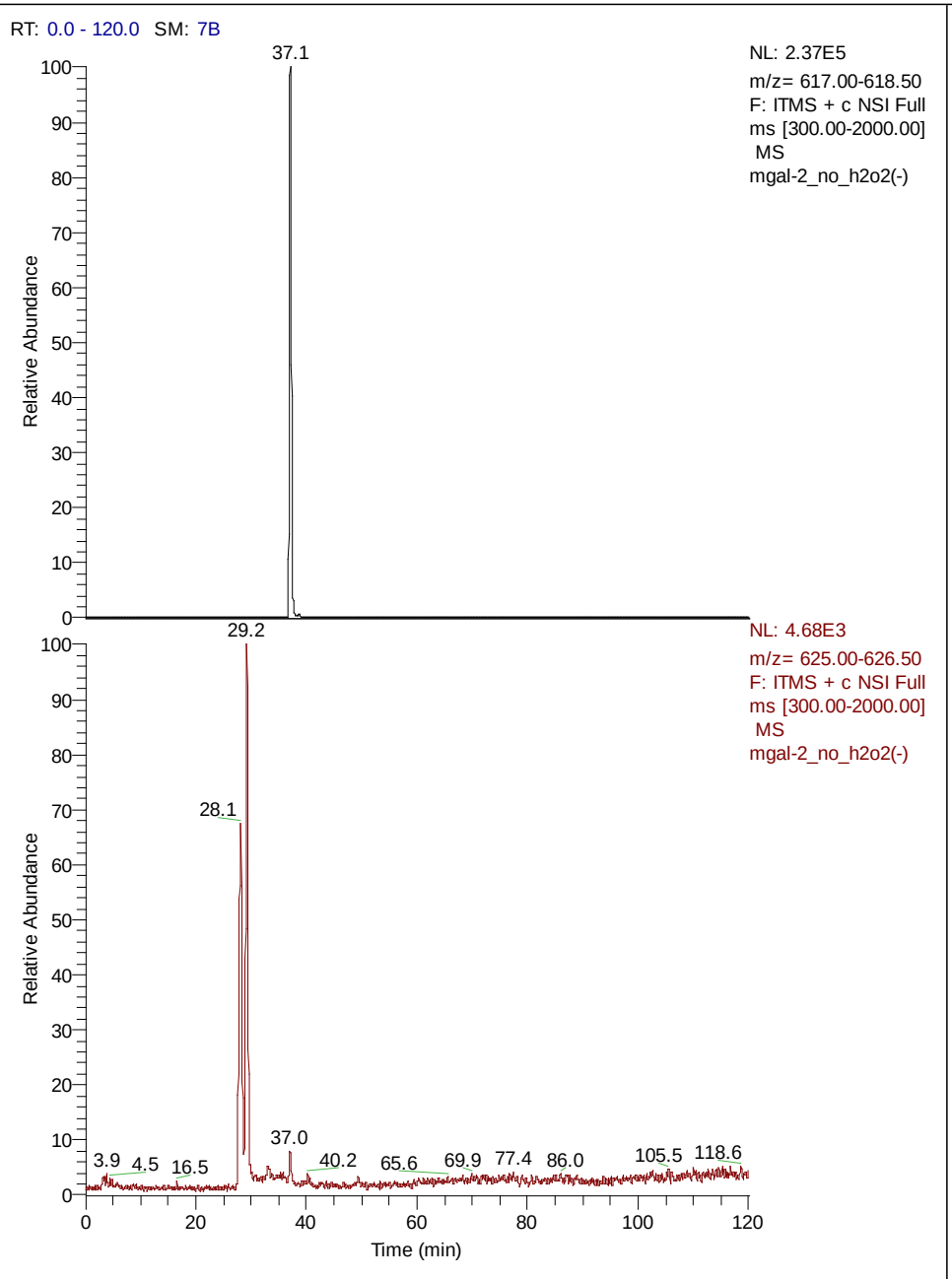


Fig. S1-E (E-1, E-2, E-3) (b). MS/MS spectra of the ions E-1, E-2, and E-3 shown in Fig. S1-E.

Fig. S1-F


RT: 0.0 - 120.0 SM: 7B
37.1
NL: 2.37E5
m/z= 617.00-618.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
Relative Abundance
29.2
NL: 4.68E3
m/z= 625.00-626.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(-)
28.1
37.0
3.9
4.5
16.5
40.2
65.6
69.9
77.4
86.0
105.5
118.6
Time (min)

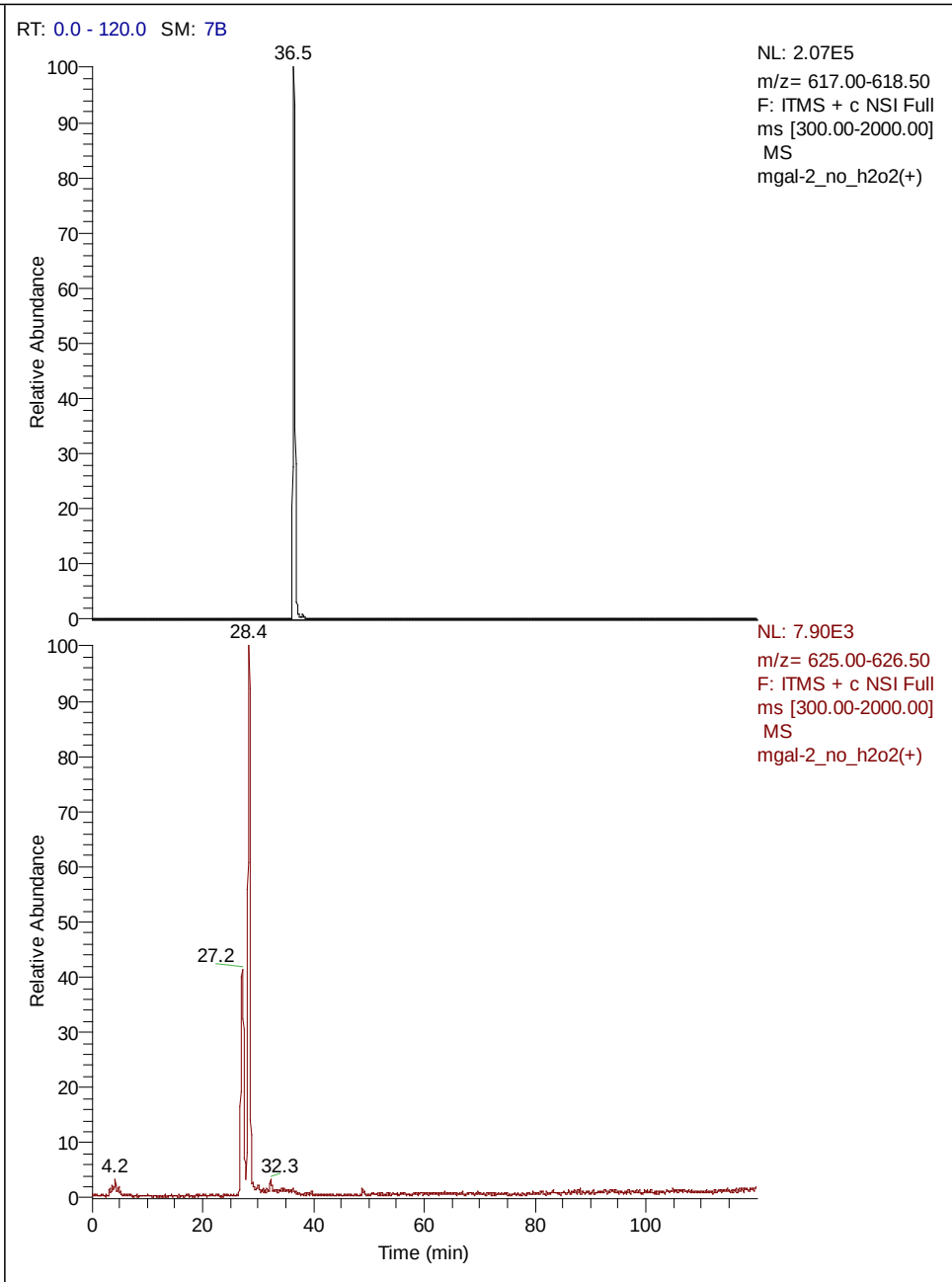

RT: 0.0 - 120.0 SM: 7B
36.5
NL: 2.07E5
m/z= 617.00-618.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
Relative Abundance
28.4
NL: 7.90E3
m/z= 625.00-626.50
F: ITMS + c NSI Full
ms [300.00-2000.00]
MS
mgal-2_no_h2o2(+)
27.2
4.2
32.3
Time (min)

Fig. S1-F. Full region of the mass chromatograms shown in Fig. 1F. Left and right columns correspond to supernatant of non-oxidized sample and oxidized sample, respectively. Upper and lower rows are LC/MS chromatograms monitoring selected peptide fragments with theoretical molecular weight expected from the sequence ($[M+2H]^{2+}$=617.32, mass range: m/z 617-618.5) and theoretical molecular weight plus 16 ($[M+O+2H]^{2+}$=625.32, mass range: m/z 625-626.5), respectively. The horizontal axis indicates retention time (min) and the vertical axis indicates relative abundance of ions.