Figure 1

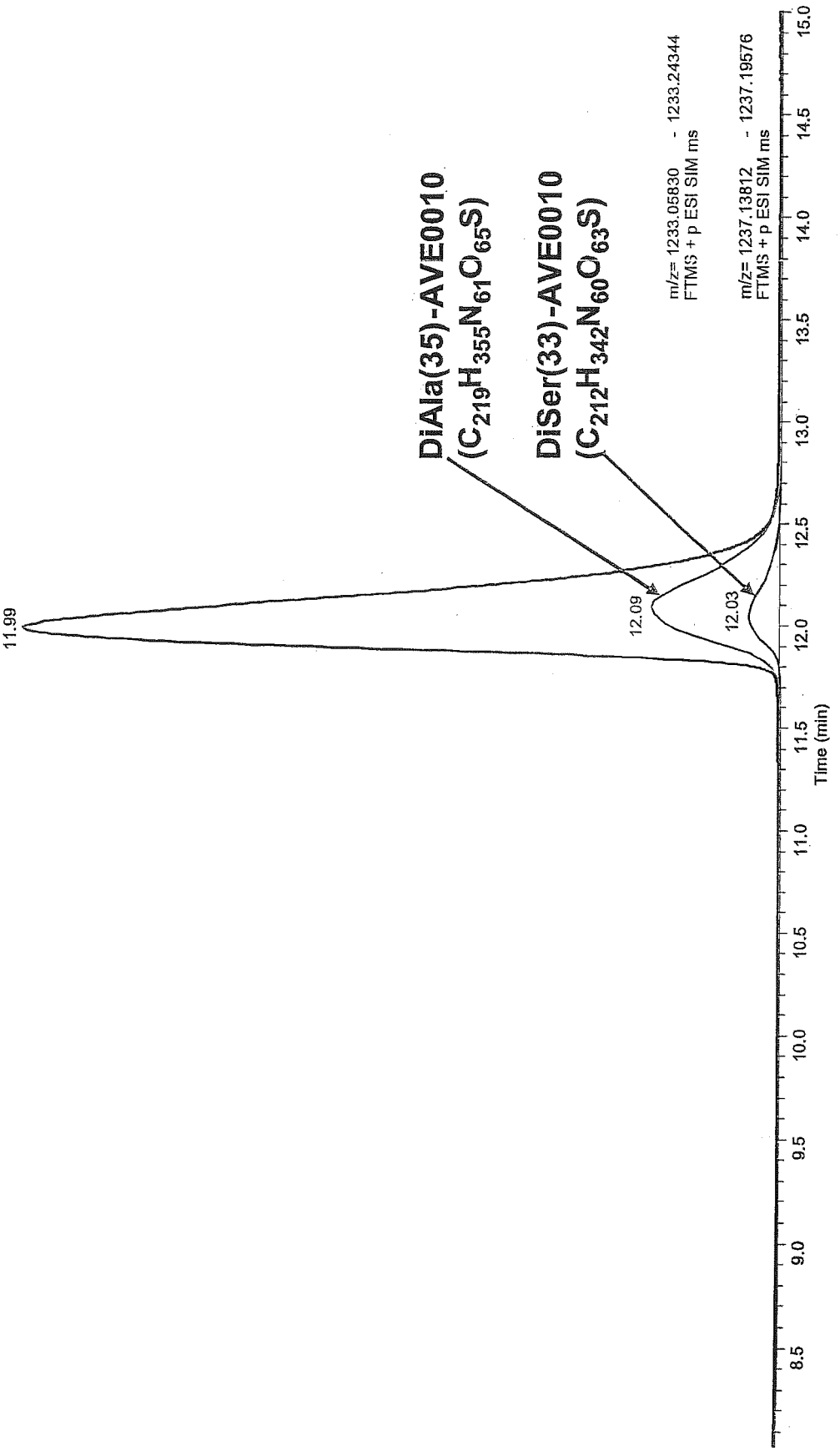

DiAla(35)-AVE0010
(C219H355N61O65S)
DiSer(33)-AVE0010
(C212H342N60O63S)
m/z= 1233.05830 - 1233.24344
FTMS + p ESI SIM ms
m/z= 1237.13812 - 1237.19576
FTMS + p ESI SIM ms
11.99
12.09
12.03
8.5
9.0
9.5
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
14.5
15.0
Time (min)

Figure 2

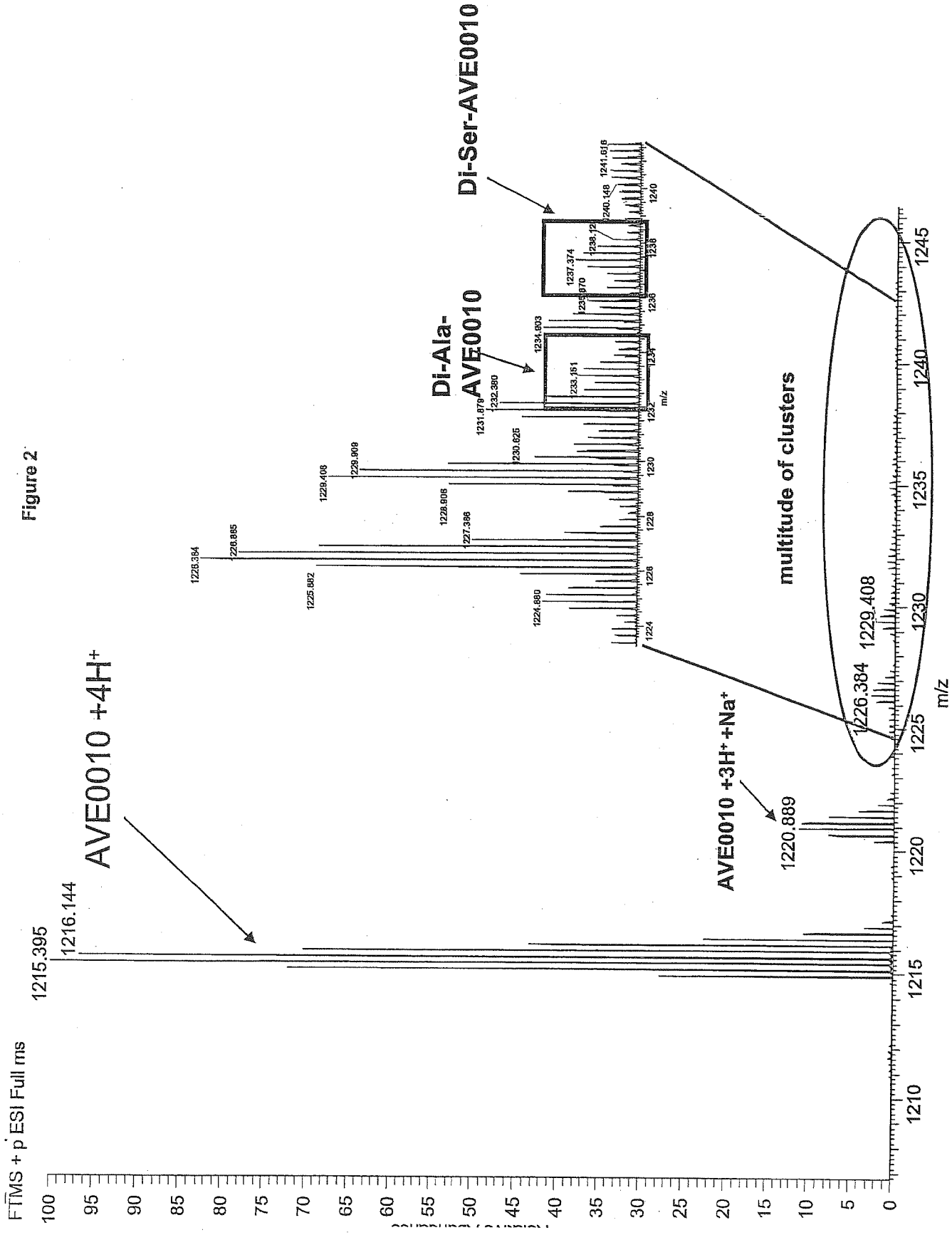

FTMS + p ESI Full ms
AVE0010 +4H+
AVE0010 +3H+ +Na+
Di-Ala-AVE0010
Di-Ser-AVE0010
multitude of clusters
m/z

Figure 3

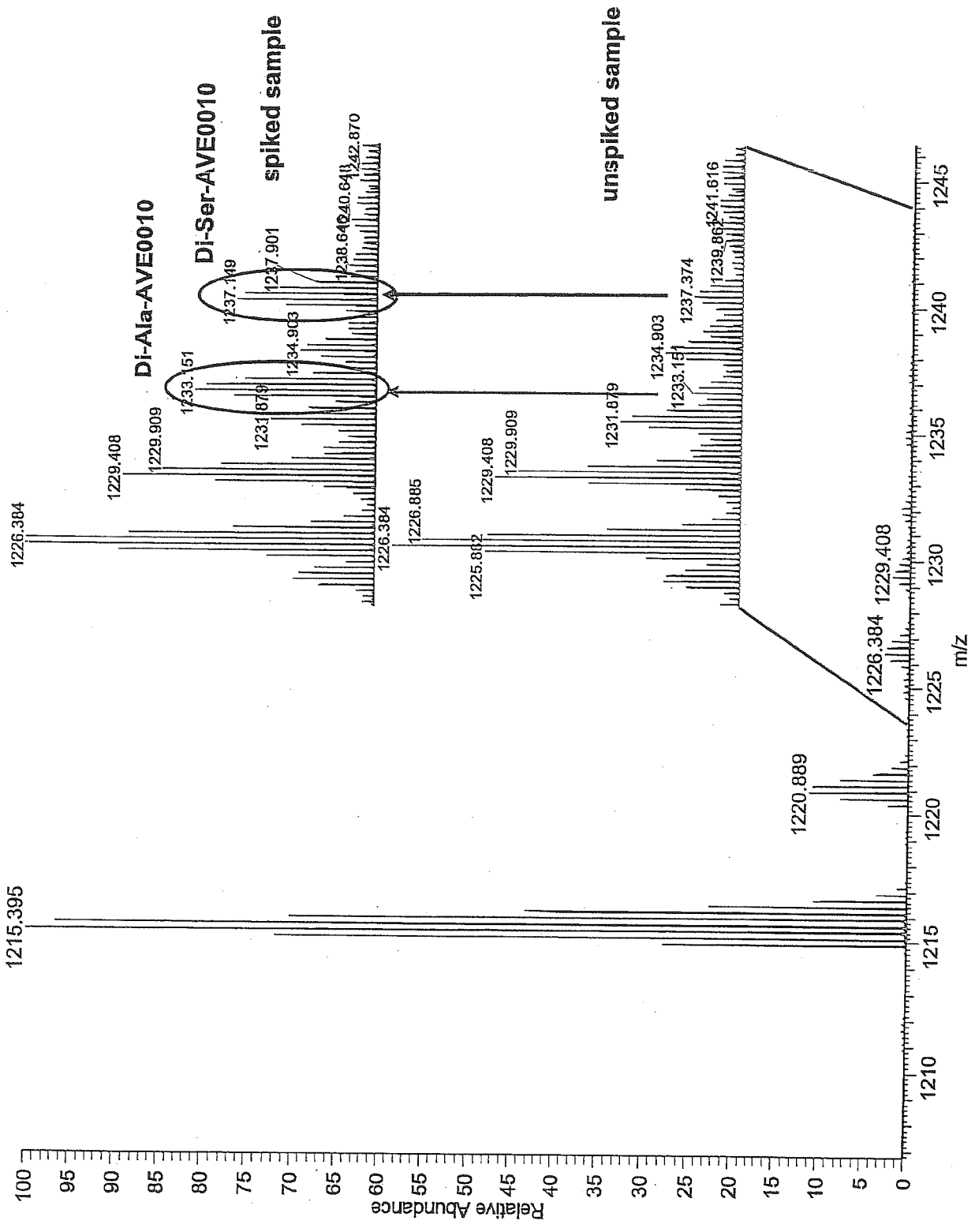

Di-Ala-AVE0010
Di-Ser-AVE0010
spiked sample
unspiked sample
Relative Abundance
m/z
1215.395
1226.384
1229.408
1229.909
1233.151
1231.879
1234.903
1237.119
1237.901
1238.640
1240.641
1242.870
1225.882
1226.885
1231.879
1233.151
1234.903
1237.374
1239.862
1241.616
1220.889
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
1210
1215
1220
1225
1230
1235
1240
1245

Figure 4

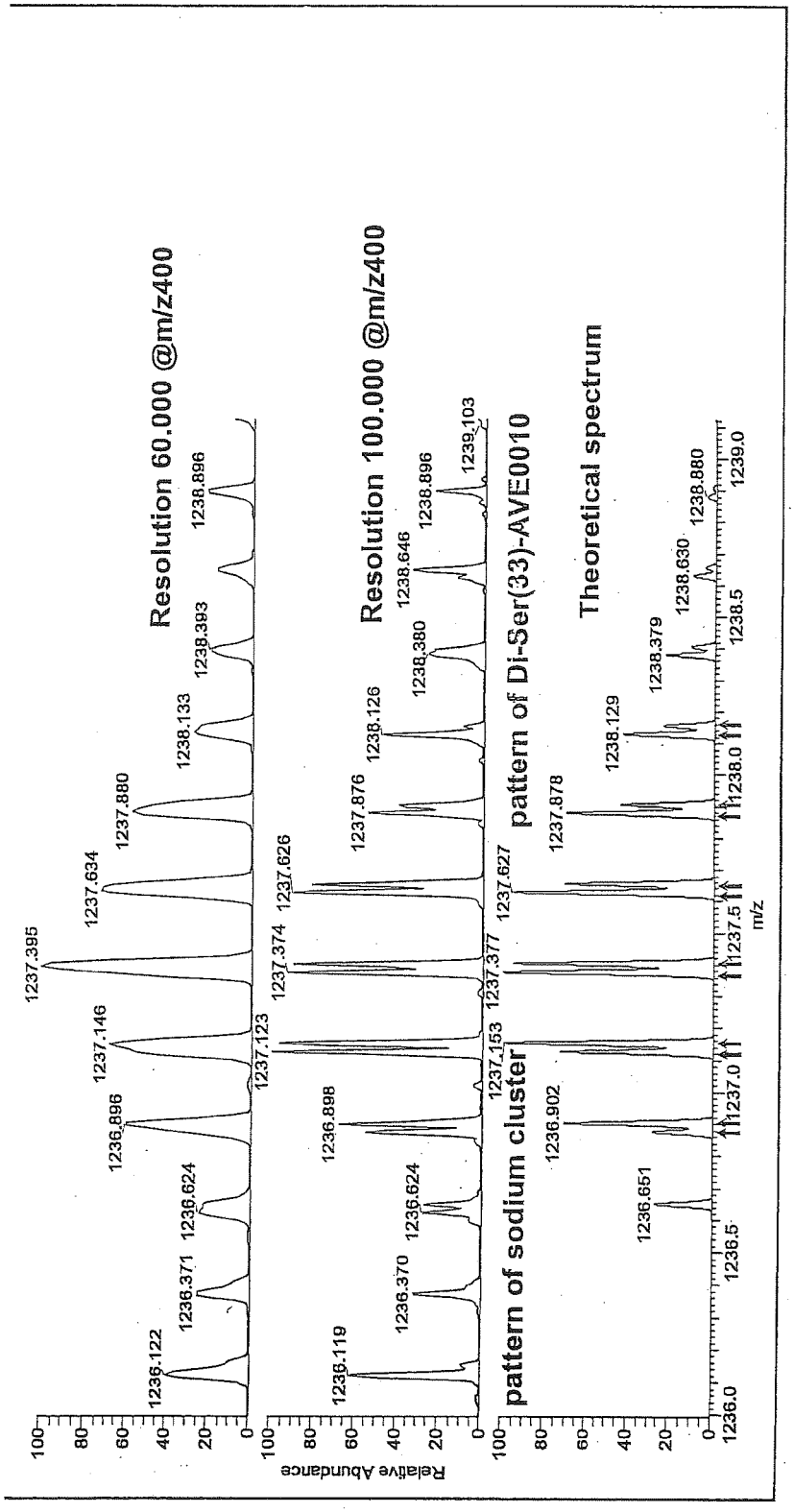

Resolution 60.000 @m/z400
Resolution 100.000 @m/z400
pattern of sodium cluster
pattern of Di-Ser(33)-AVE0010
Theoretical spectrum
Relative Abundance
m/z
1236.122
1236.371
1236.624
1236.896
1237.146
1237.395
1237.634
1237.880
1238.133
1238.393
1238.896
1238.119
1236.370
1236.624
1236.898
1237.123
1237.374
1237.626
1237.876
1238.126
1238.380
1238.646
1238.896
1239.103
1236.651
1236.902
1237.153
1237.377
1237.627
1237.878
1238.129
1238.379
1238.630
1238.880
1236.0
1236.5
1237.0
1237.5
1238.0
1238.5
1239.0

Figure 5

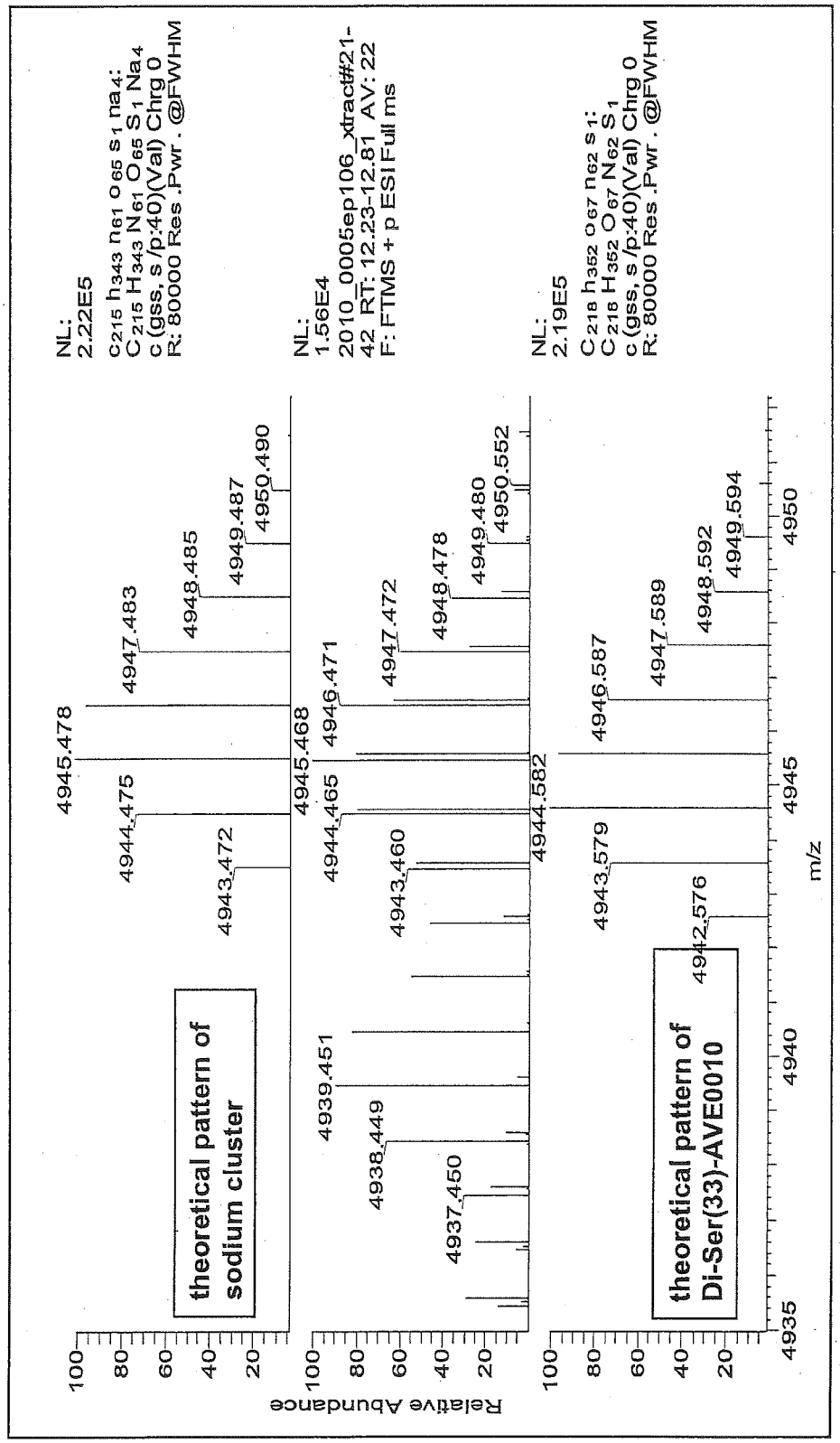
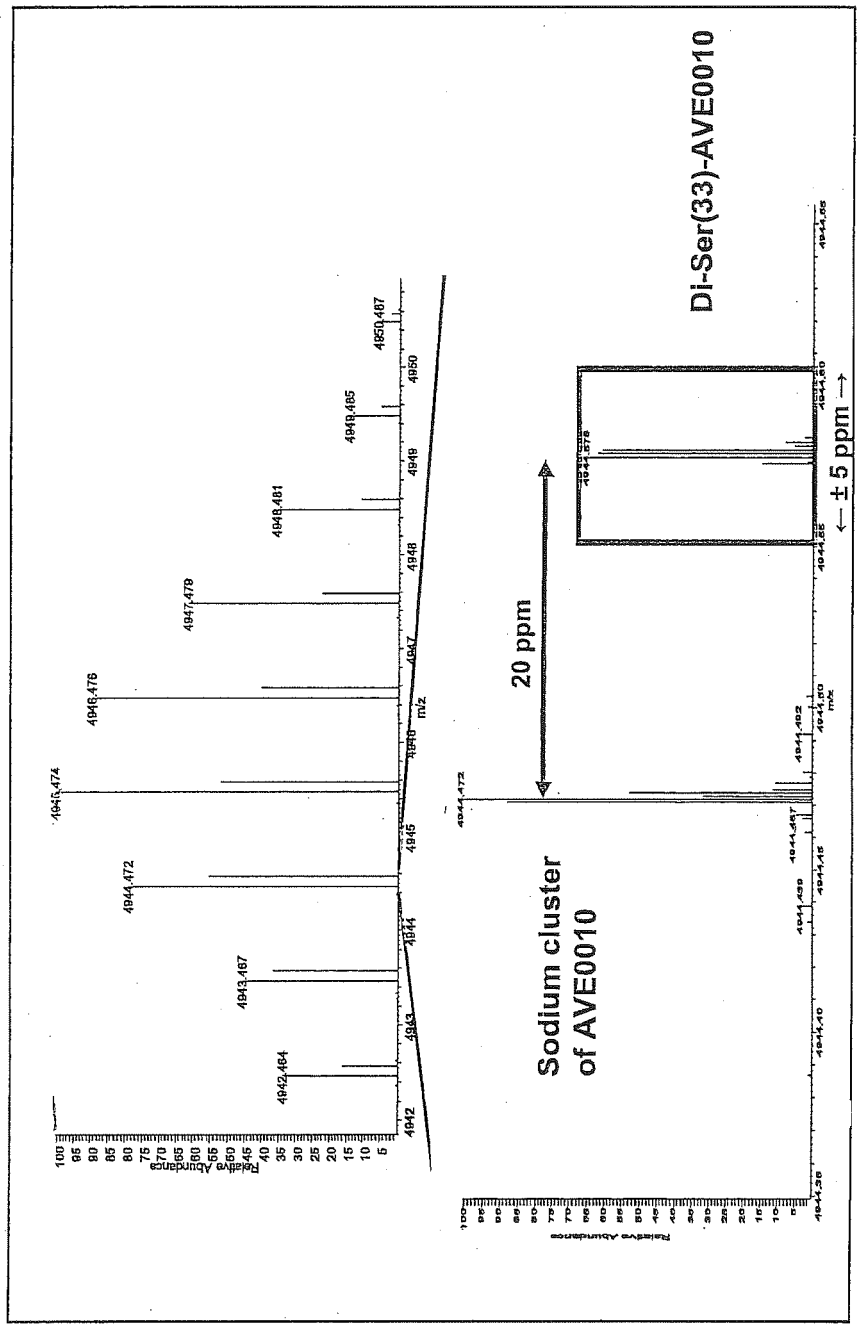
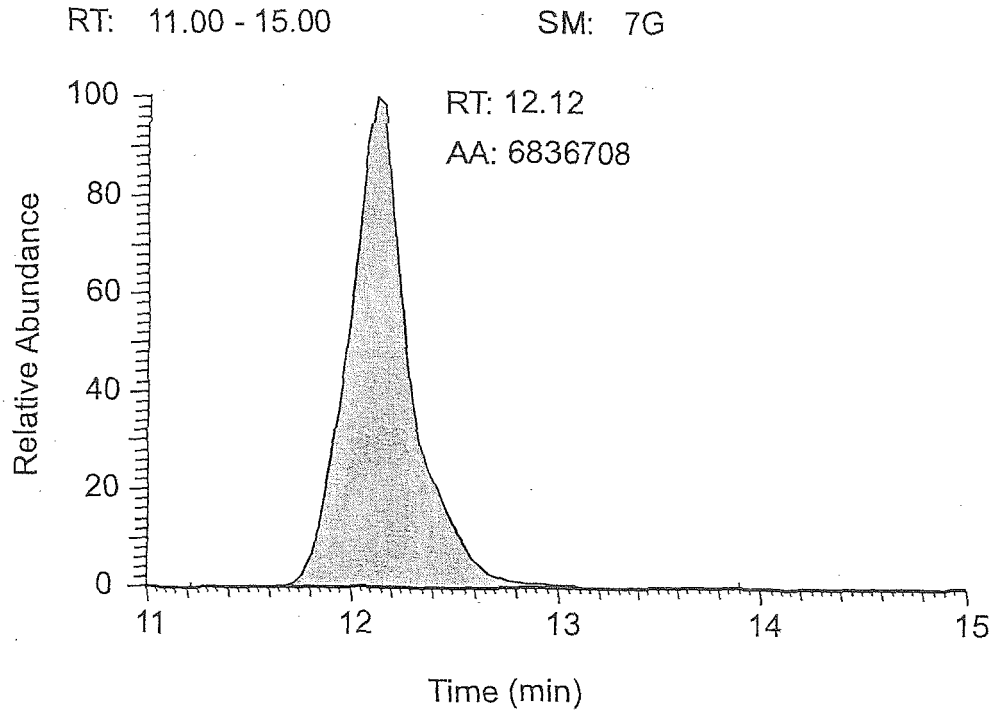
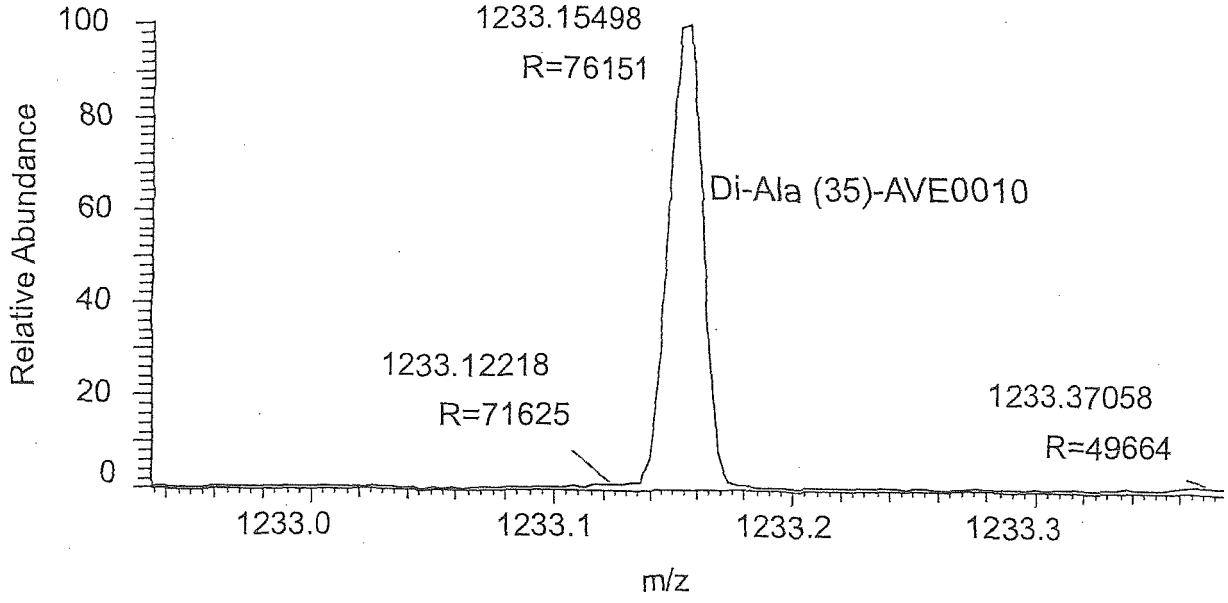
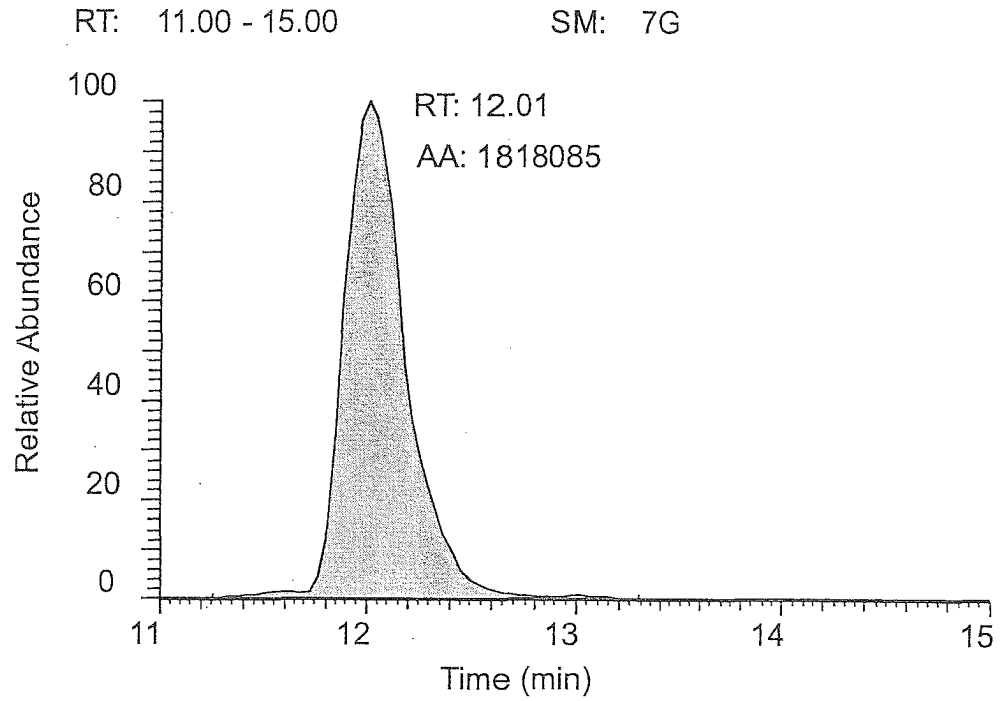

NL:
2.22E5
C215 H343 N61 O65 S1 Na4:
C215 H343 N61 O65 S1 Na4
c (gss, s /p:40)(Val) Chrg 0
R: 80000 Res .Pwr. @FWHM
NL:
1.56E4
2010_0005ep106_xtract#21-42 RT: 12.23-12.81 AV: 22
F: FTMS + p ESI Full ms
NL:
2.19E5
C218 H352 O67 N62 S1:
C218 H352 O67 N62 S1
c (gss, s /p:40)(Val) Chrg 0
R: 80000 Res .Pwr. @FWHM
theoretical pattern of sodium cluster
theoretical pattern of Di-Ser(33)-AVE0010
Relative Abundance
m/z
4935
4940
4945
4950
4937.450
4938.449
4939.451
4942.576
4943.460
4943.472
4943.579
4944.465
4944.475
4944.582
4945.468
4945.478
4946.471
4946.587
4947.472
4947.483
4947.589
4948.478
4948.485
4948.592
4949.480
4949.487
4949.594
4950.490
4950.552

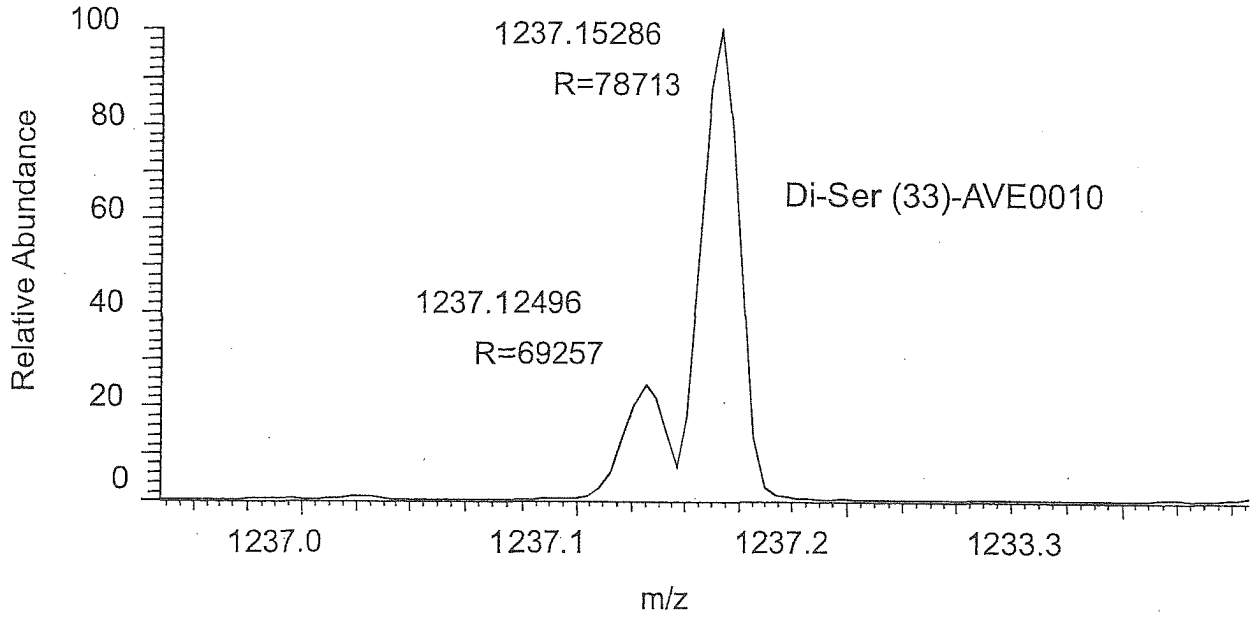
Figure 6

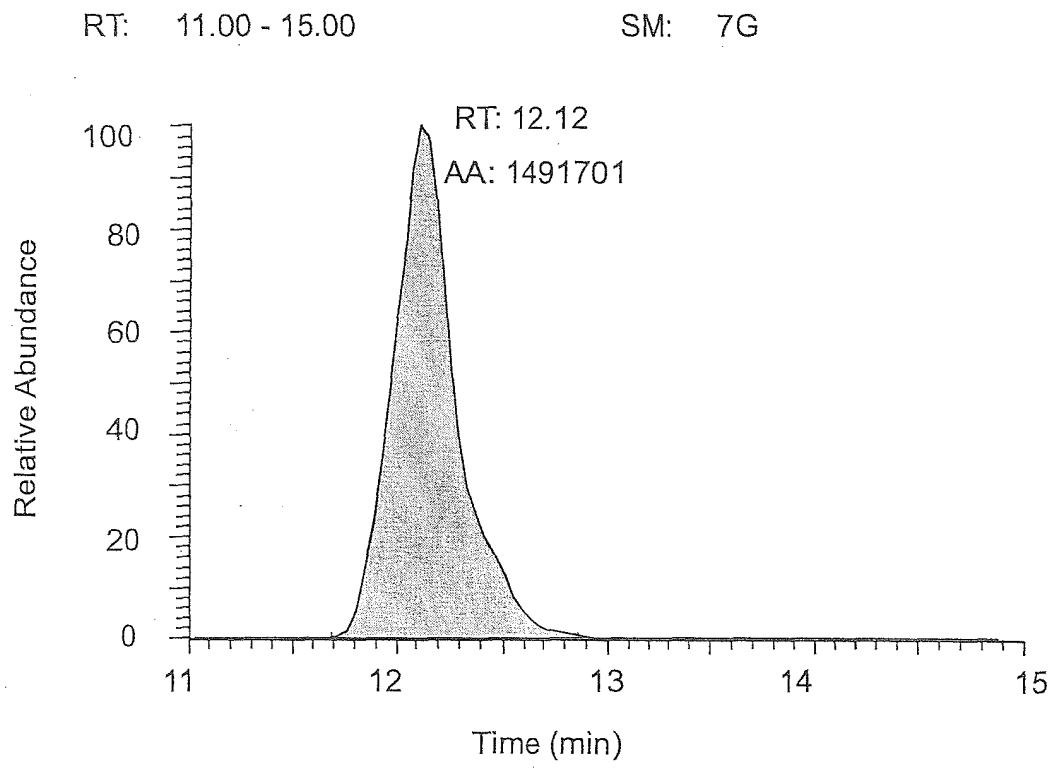

Di-Ser(33)-AVE0010
Sodium cluster of AVE0010
20 ppm
← ± 5 ppm →
Relative Abundance
m/z
4942,464
4943,467
4944,472
4945,474
4946,476
4947,479
4948,481
4949,485
4950,487

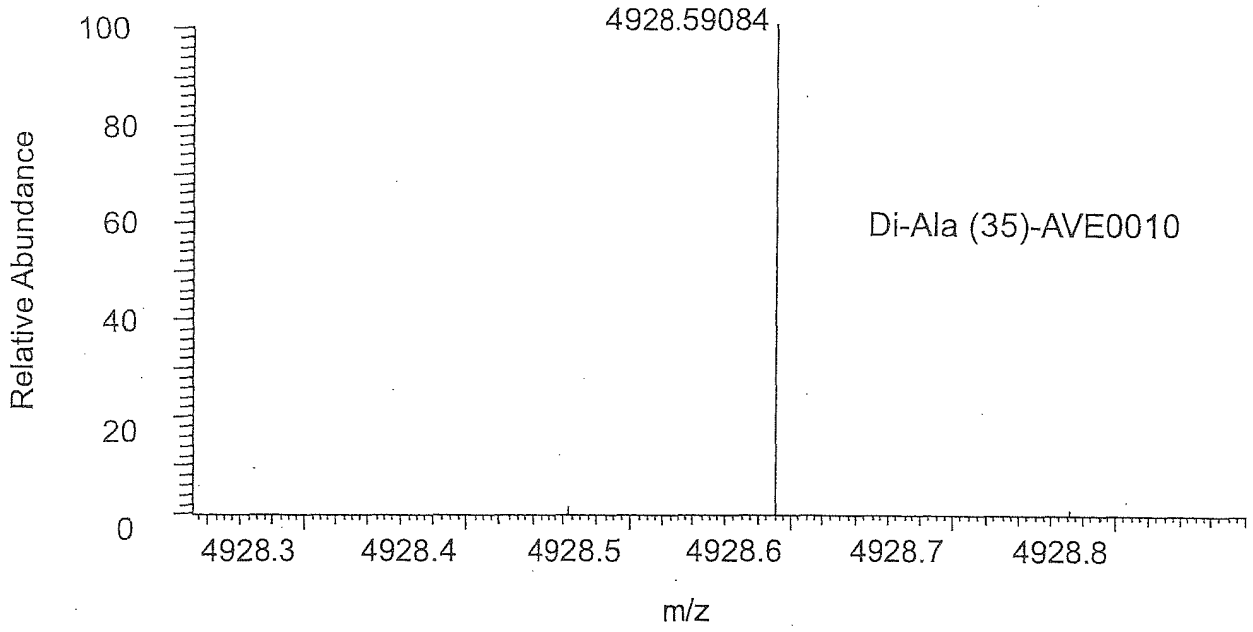

RT: 11.00 - 15.00
SM: 7G
RT: 12.12
AA: 6836708
Relative Abundance
100
80
60
40
20
0
11
12
13
14
15
Time (min)

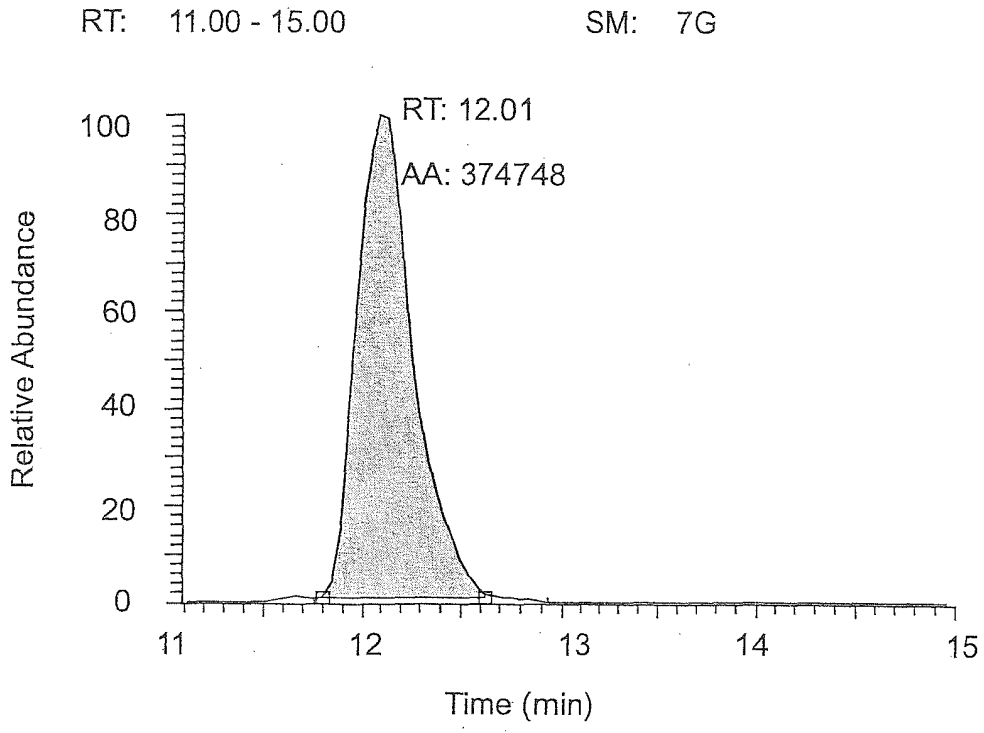

1233.15498
R=76151
Di-Ala (35)-AVE0010
1233.12218
R=71625
1233.37058
R=49664
Relative Abundance
100
80
60
40
20
0
1233.0
1233.1
1233.2
1233.3
m/z


RT: 11.00 - 15.00
SM: 7G
RT: 12.01
AA: 1818085
Relative Abundance
Time (min)
100
80
60
40
20
0
11
12
13
14
15


1237.15286
R=78713
Di-Ser (33)-AVE0010
1237.12496
R=69257
Relative Abundance
m/z
100
80
60
40
20
0
1237.0
1237.1
1237.2
1233.3


RT: 11.00 - 15.00
SM: 7G
RT: 12.12
AA: 1491701
Relative Abundance
Time (min)
100
80
60
40
20
0
11
12
13
14
15


4928.59084
Di-Ala (35)-AVE0010
Relative Abundance
m/z
100
80
60
40
20
0
4928.3
4928.4
4928.5
4928.6
4928.7
4928.8


RT: 11.00 - 15.00
SM: 7G
RT: 12.01
AA: 374748
Relative Abundance
100
80
60
40
20
0
11
12
13
14
15
Time (min)

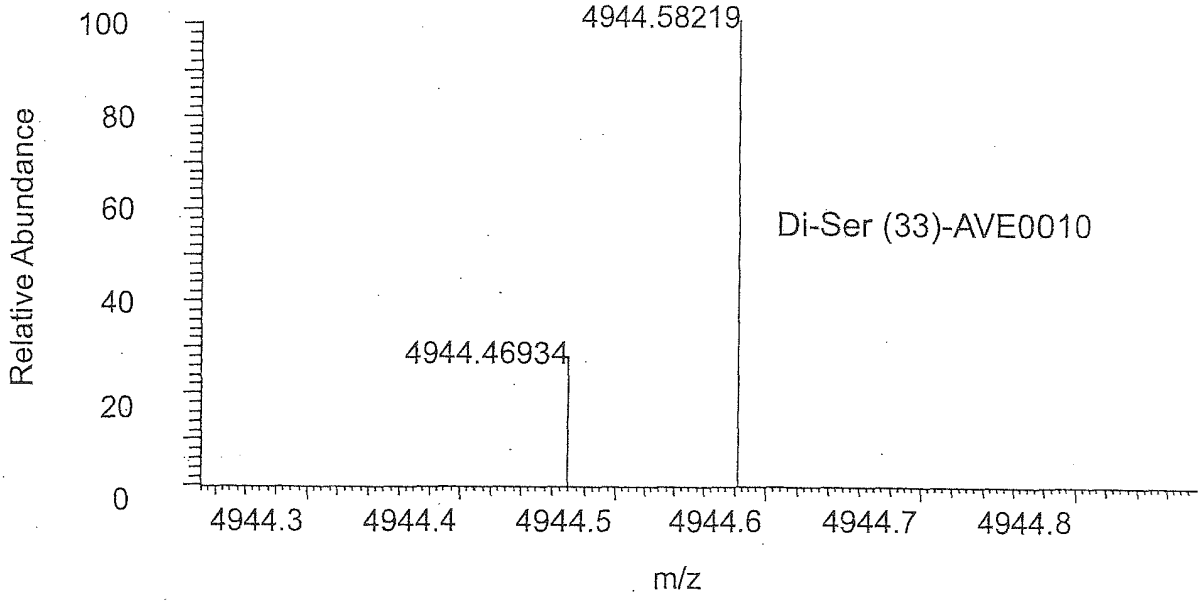
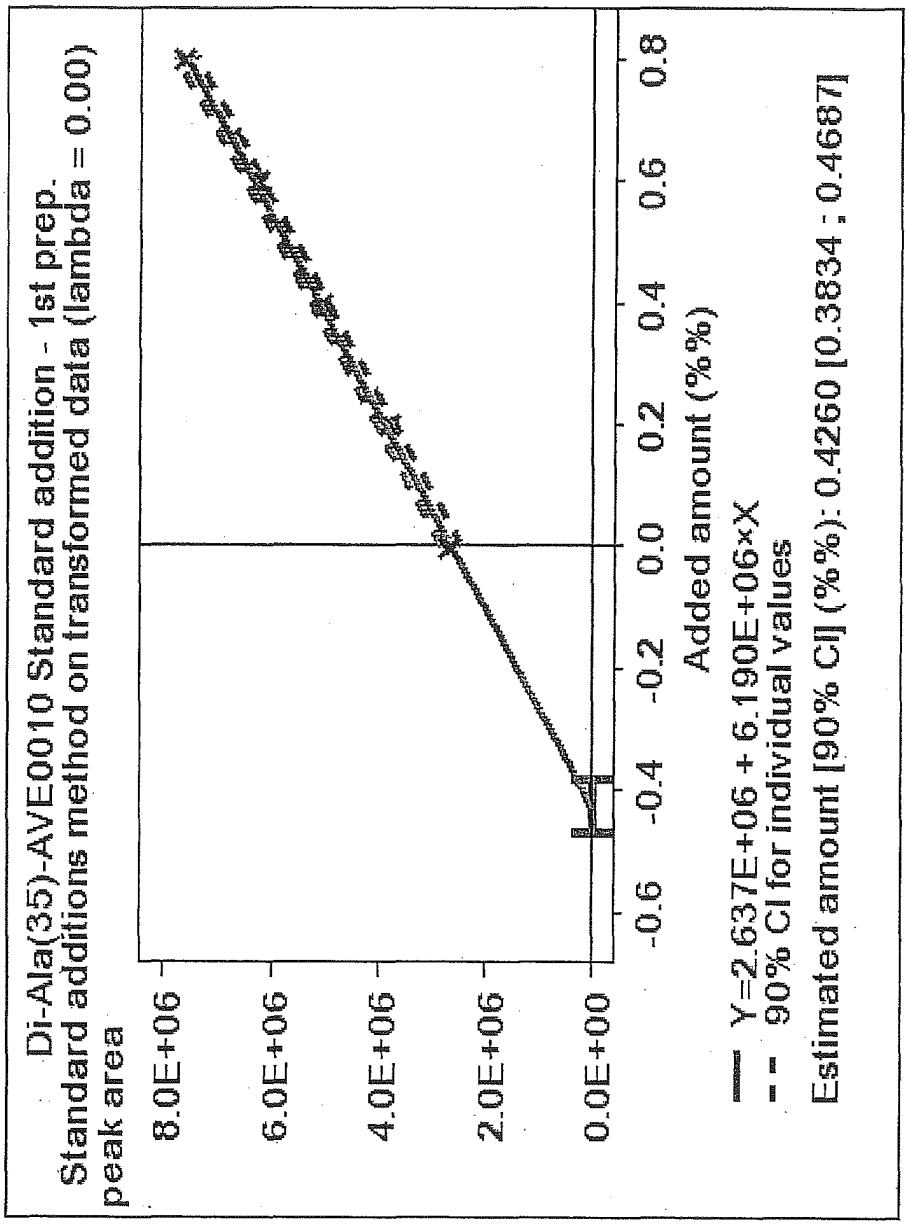

4944.58219
Di-Ser (33)-AVE0010
4944.46934
Relative Abundance
100
80
60
40
20
0
4944.3
4944.4
4944.5
4944.6
4944.7
4944.8
m/z

Figure 9


Di-Ala(35)-AVE0010 Standard addition - 1st prep.
Standard additions method on transformed data (lambda = 0.00)
peak area
8.0E+06
6.0E+06
4.0E+06
2.0E+06
0.0E+00
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
0.8
Added amount (%%)
Y=2.637E+06 + 6.190E+06*X
90% CI for individual values
Estimated amount [90% CI] (%%): 0.4260 [0.3834 ; 0.4687]