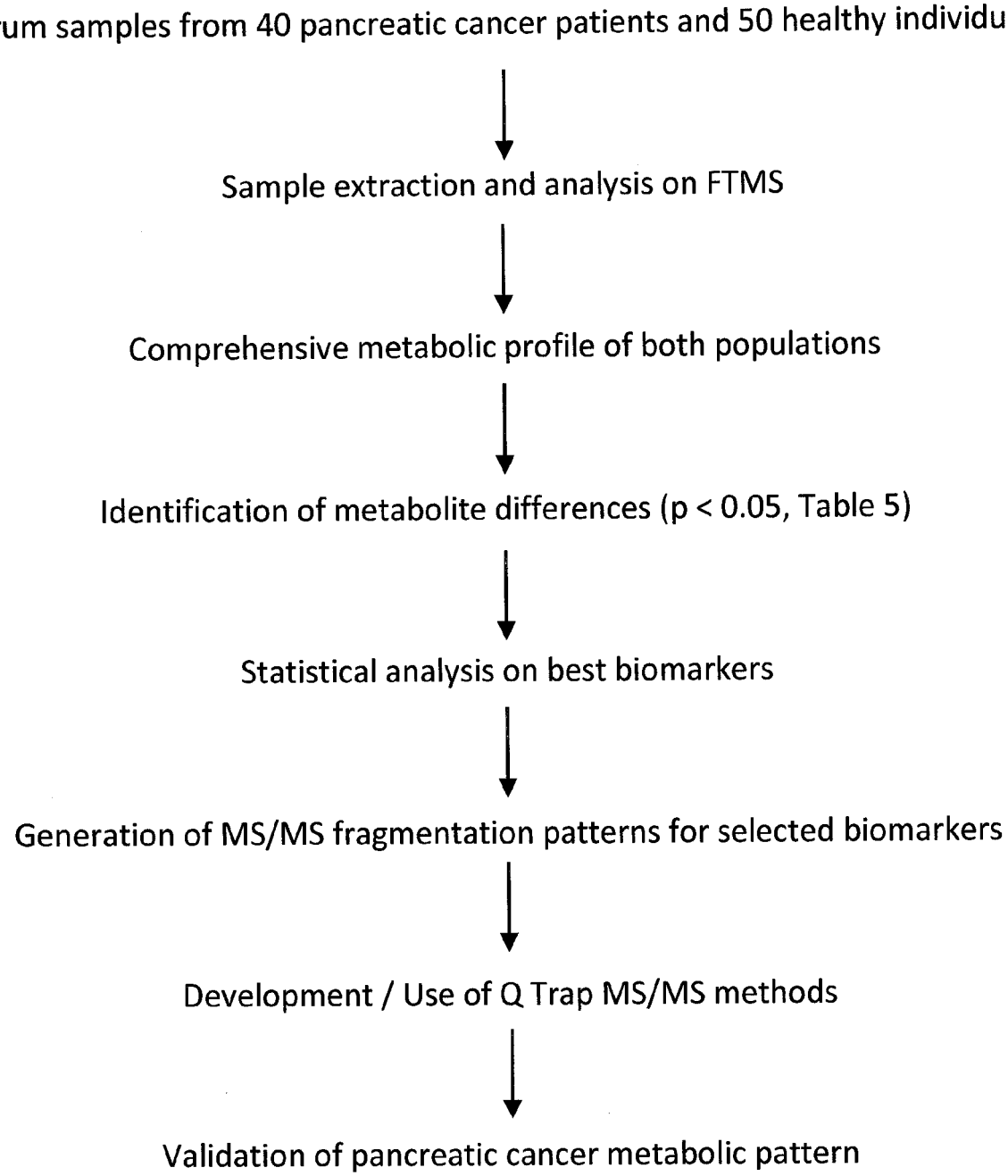

Serum samples from 40 pancreatic cancer patients and 50 healthy individuals
Sample extraction and analysis on FTMS
Comprehensive metabolic profile of both populations
Identification of metabolite differences (p < 0.05, Table 5)
Statistical analysis on best biomarkers
Generation of MS/MS fragmentation patterns for selected biomarkers
Development / Use of Q Trap MS/MS methods
Validation of pancreatic cancer metabolic pattern

Figure 1

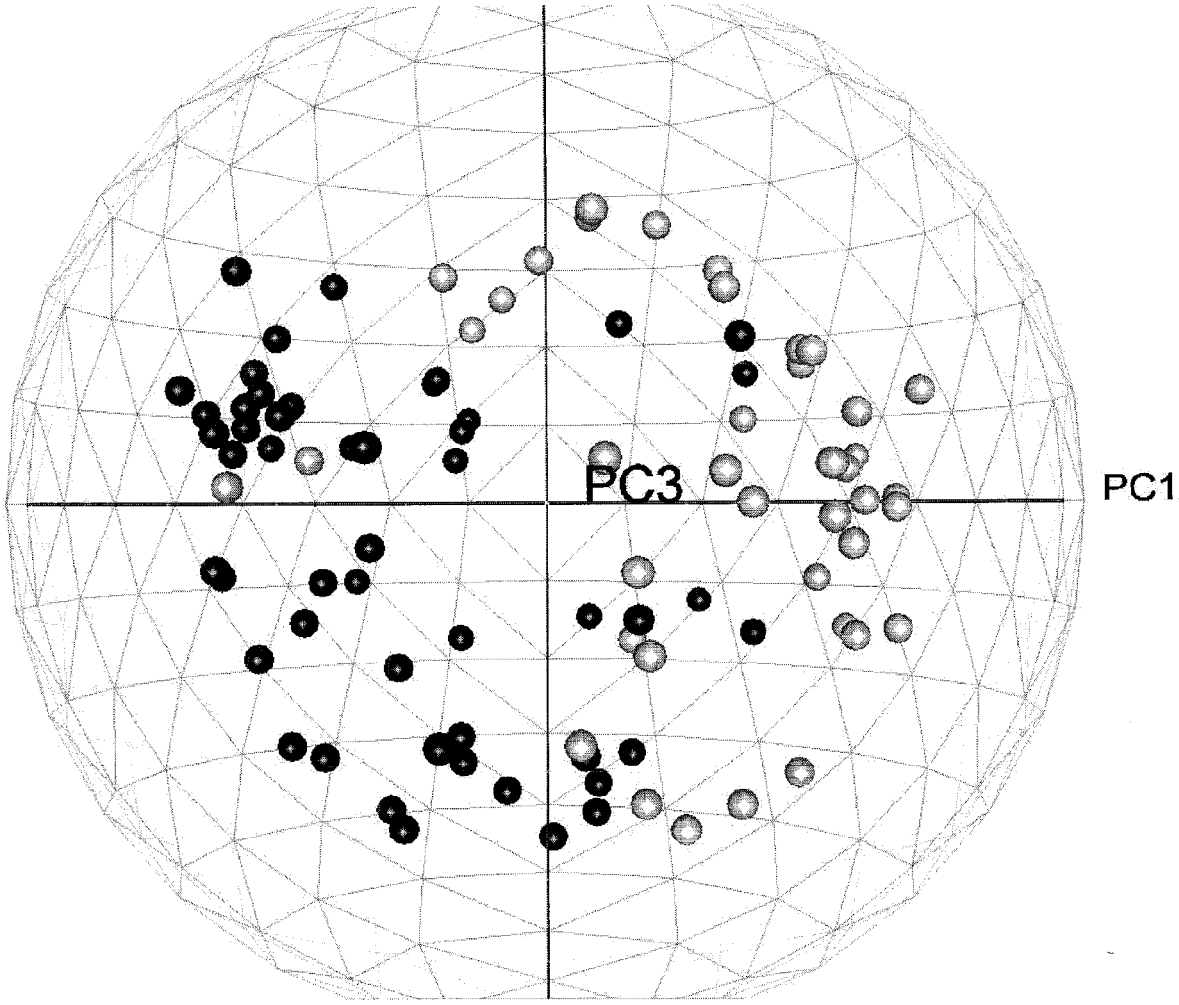


Figure 2

a)

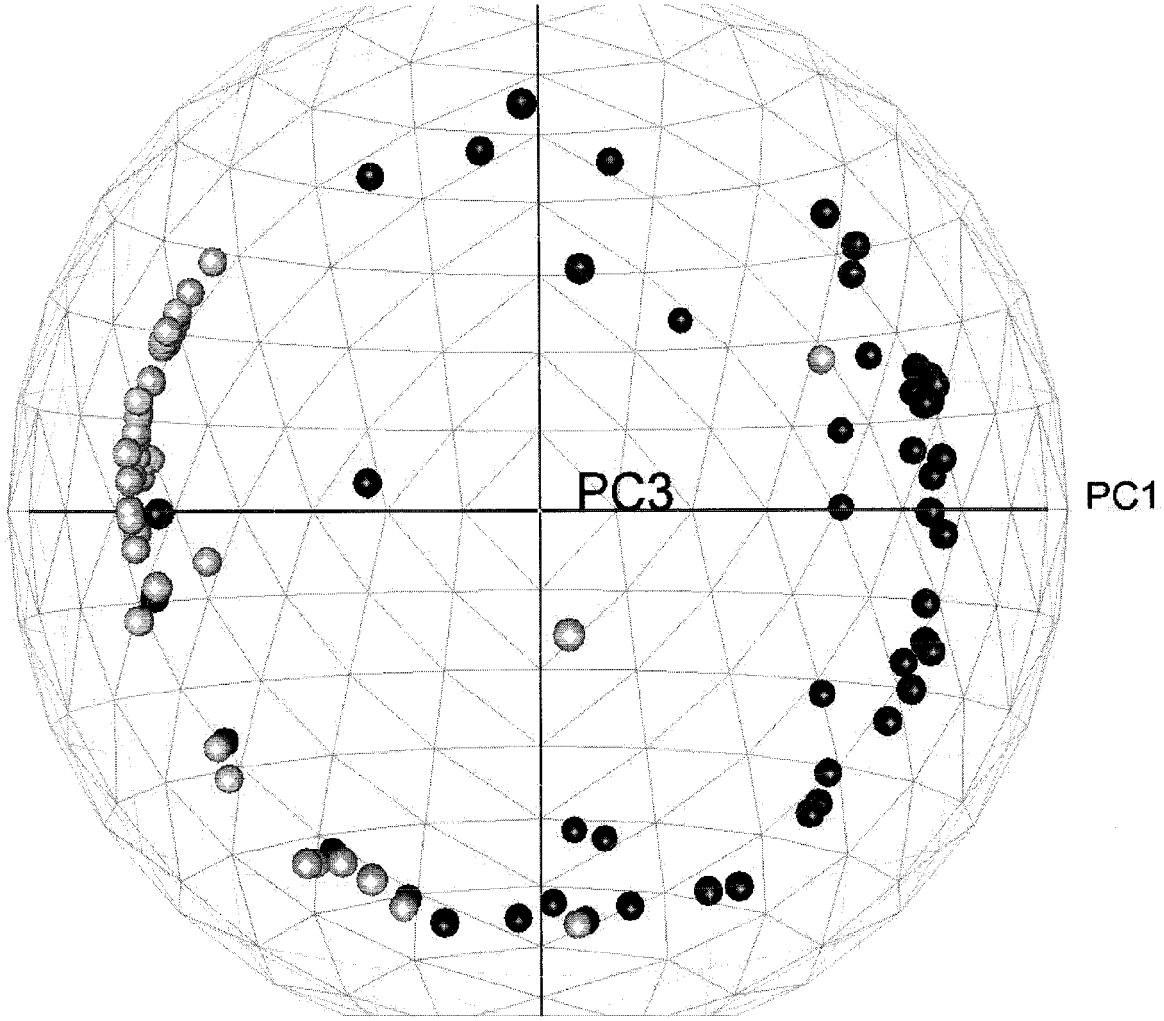
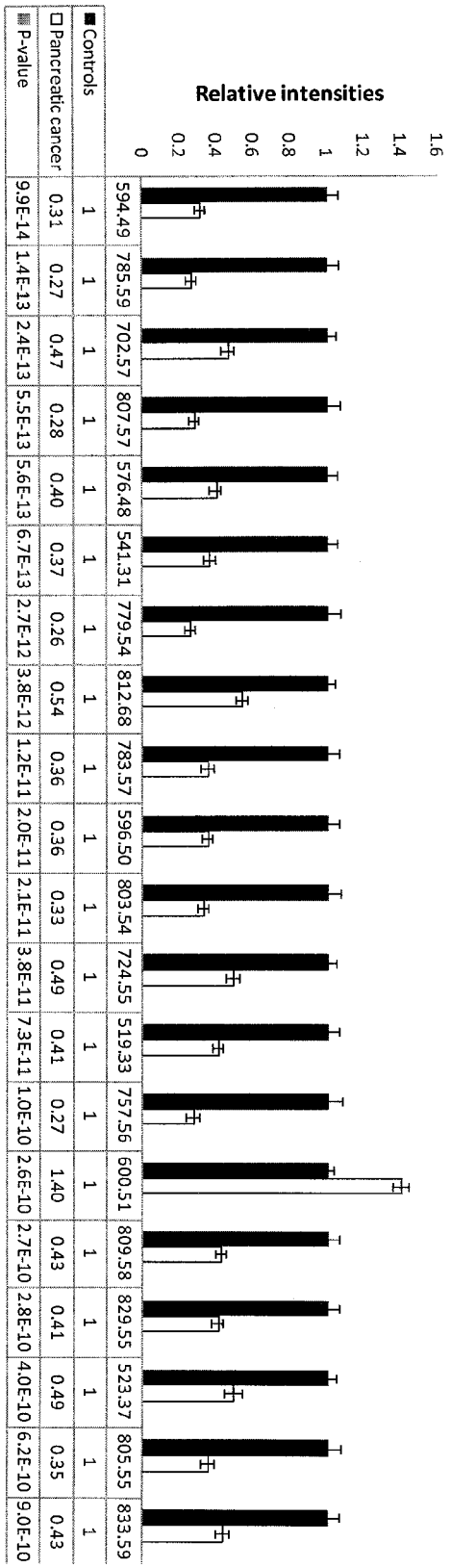


Figure 3

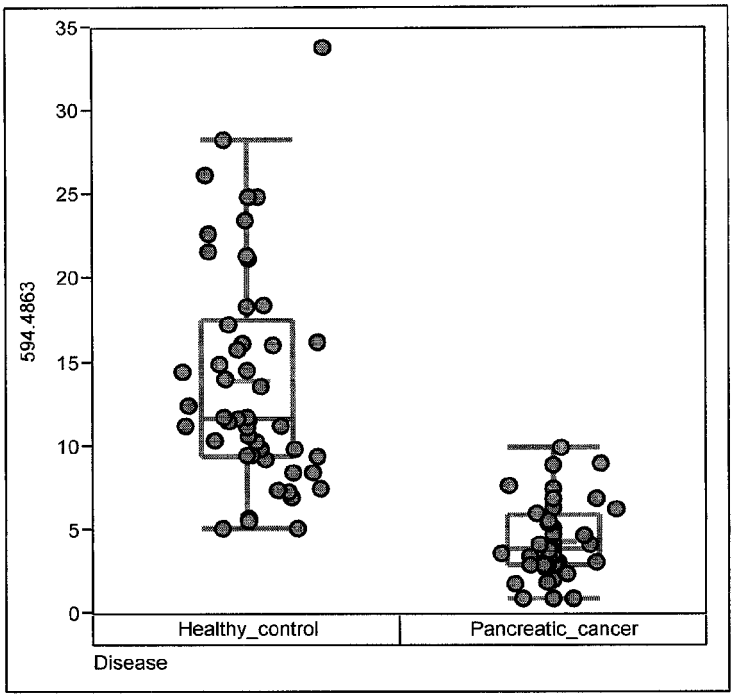
b)



	594.49	785.59	702.57	807.57	576.48	541.31	779.54	812.68	783.57	596.50	803.54	724.55	519.33	757.56	600.51	809.58	829.55	523.37	805.55	833.59
Controls	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Pancreatic cancer	0.31	0.27	0.47	0.28	0.40	0.37	0.26	0.54	0.36	0.36	0.33	0.49	0.41	0.27	1.40	0.43	0.41	0.49	0.35	0.43
P-value	9.9E-14	1.4E-13	2.4E-13	5.5E-13	5.6E-13	6.7E-13	2.7E-12	3.8E-12	1.2E-11	2.0E-11	2.1E-11	3.8E-11	7.3E-11	1.0E-10	2.6E-10	2.7E-10	2.8E-10	4.0E-10	6.2E-10	9.0E-10

Figure 3 (Cont.)

(a)


35
30
25
20
15
10
5
0
594.4863
Healthy_control
Pancreatic_cancer
Disease

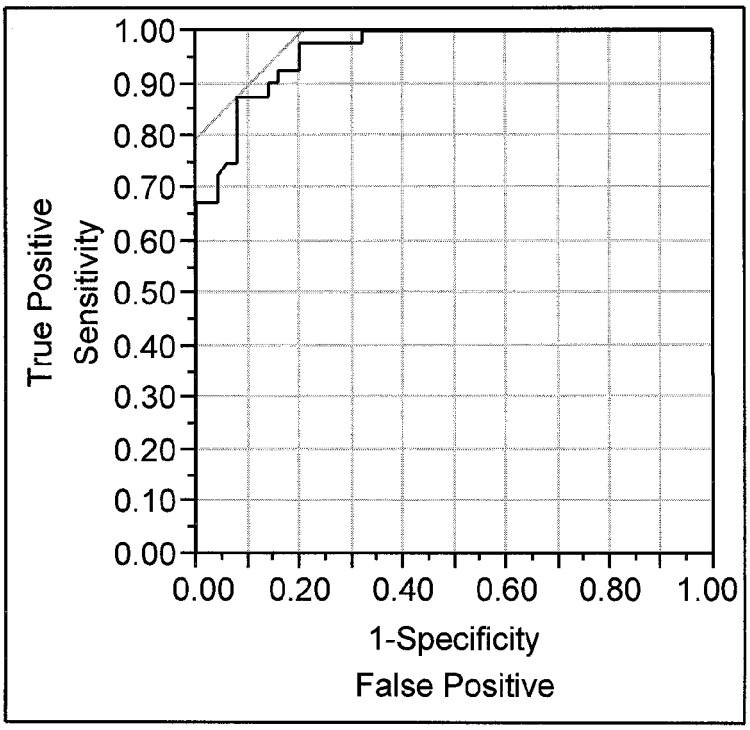
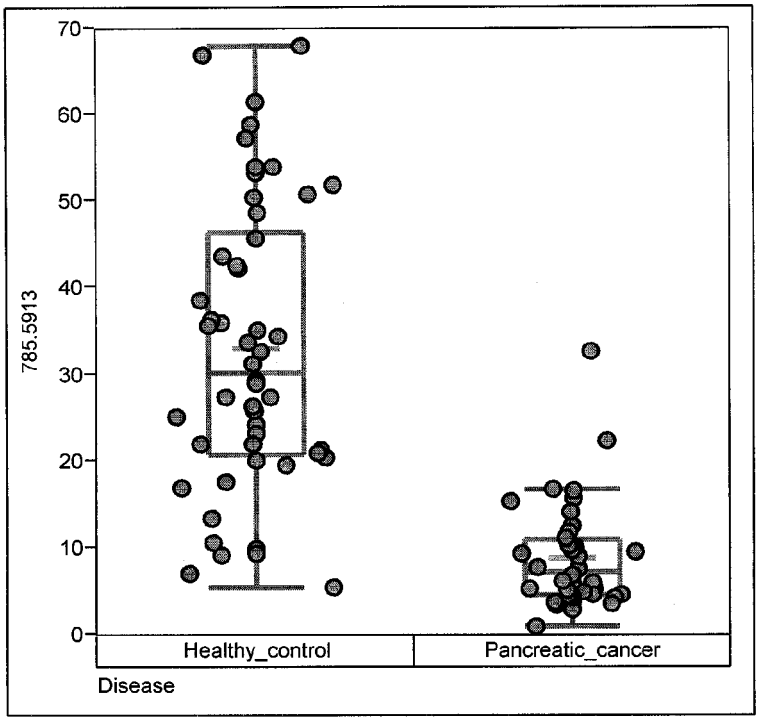

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
True Positive
Sensitivity
0.00
0.20
0.40
0.60
0.80
1.00
1-Specificity
False Positive

Figure 4

(b)



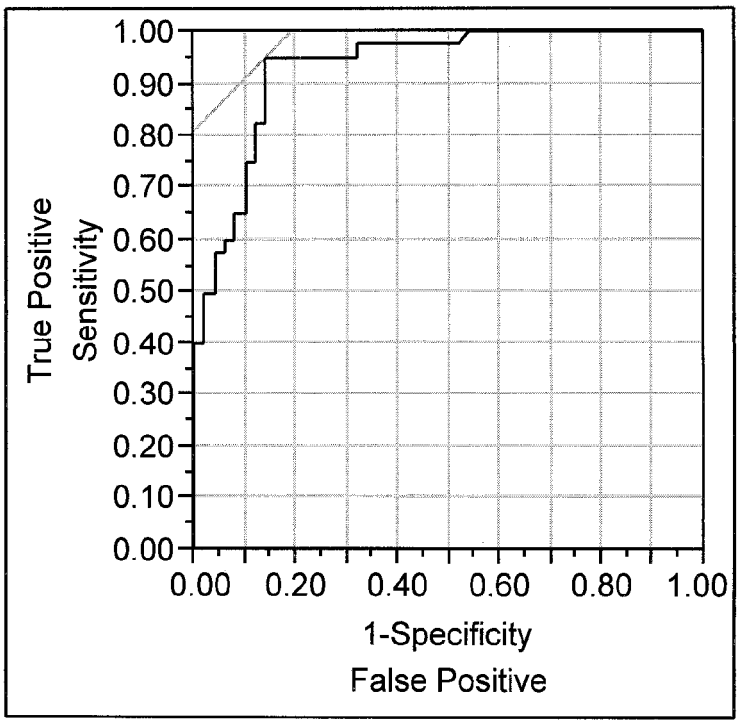
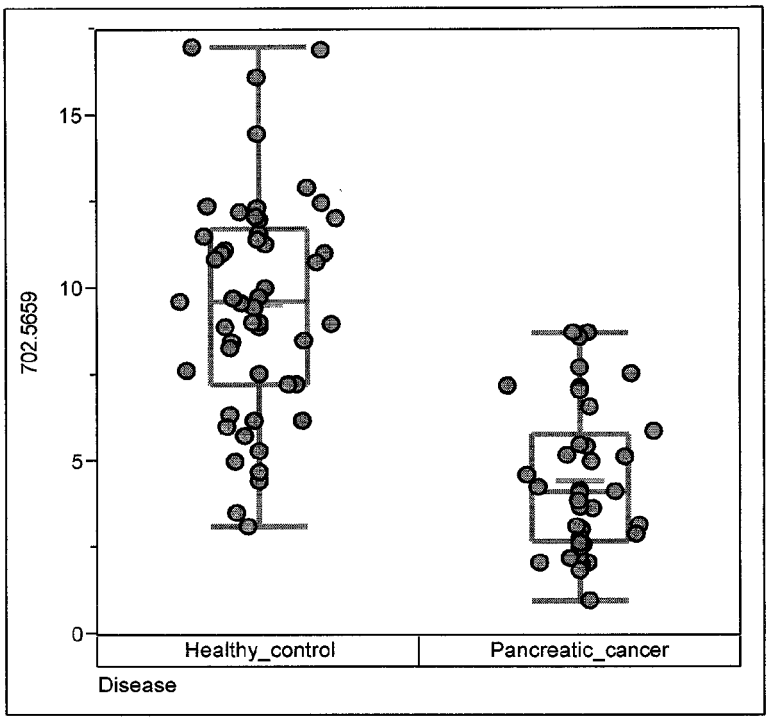


Figure 4 (cont.)

(c)



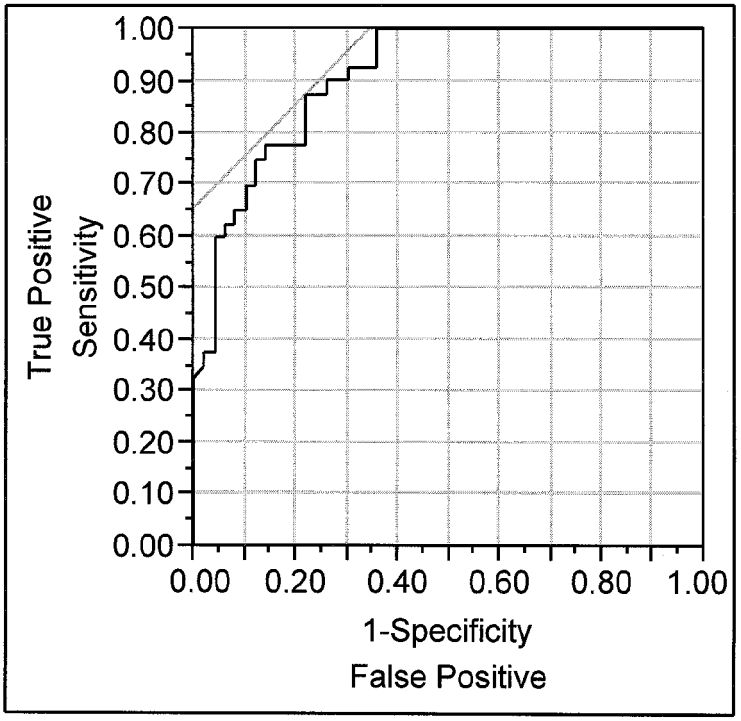
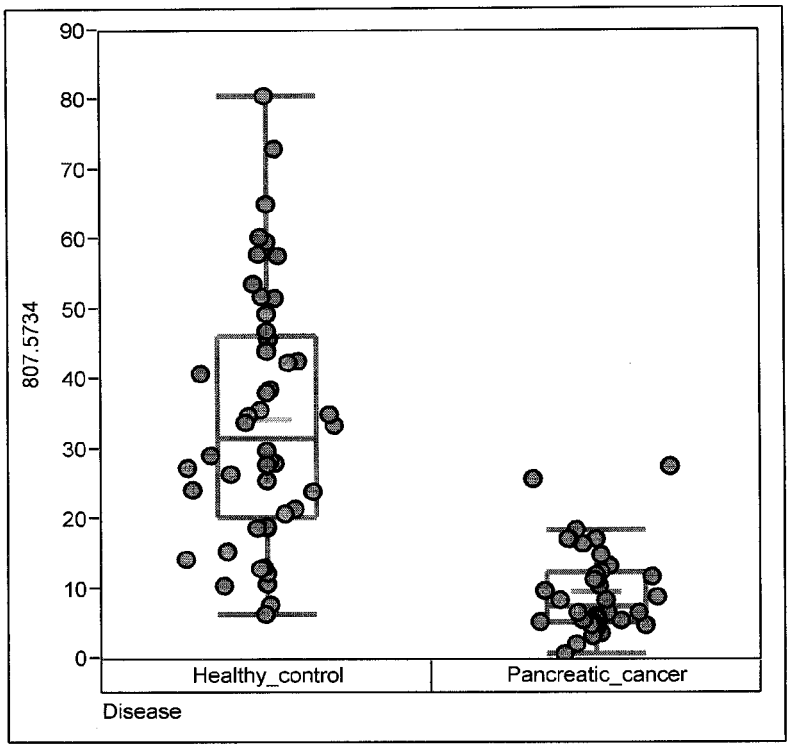


Figure 4 (cont.)

(d)



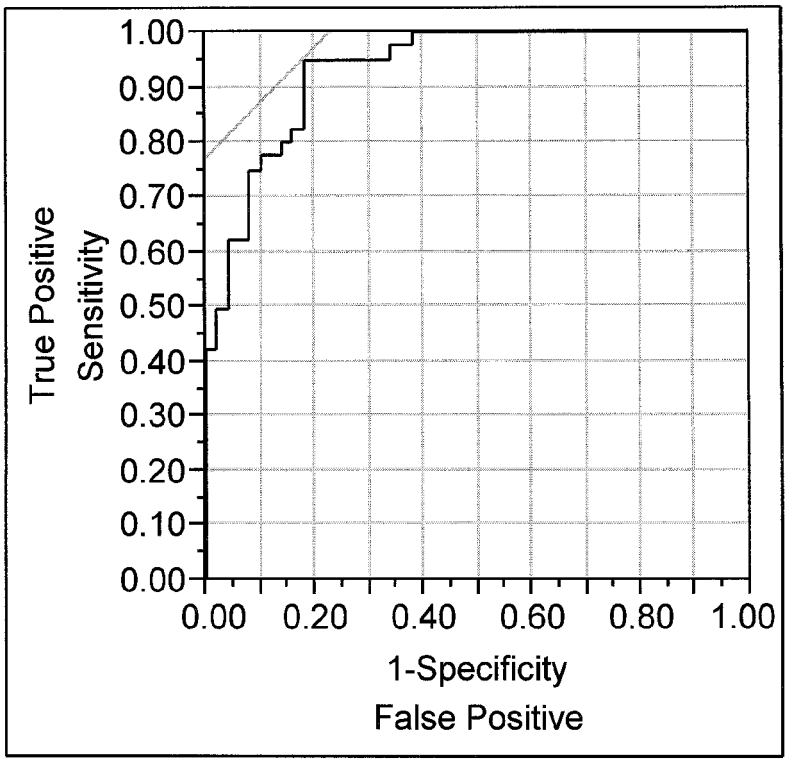
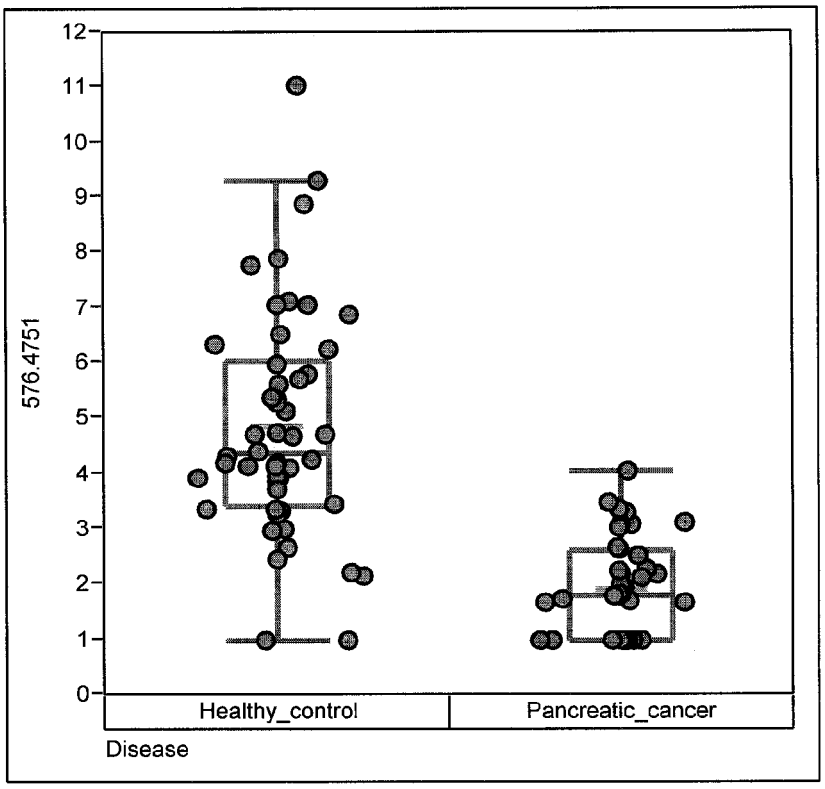


Figure 4 (cont.)

(e)



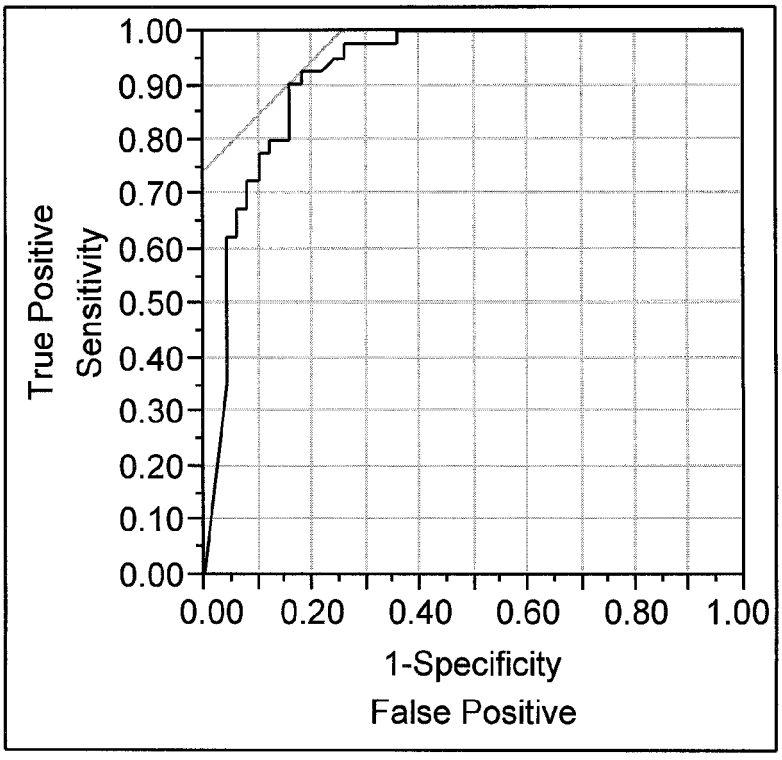
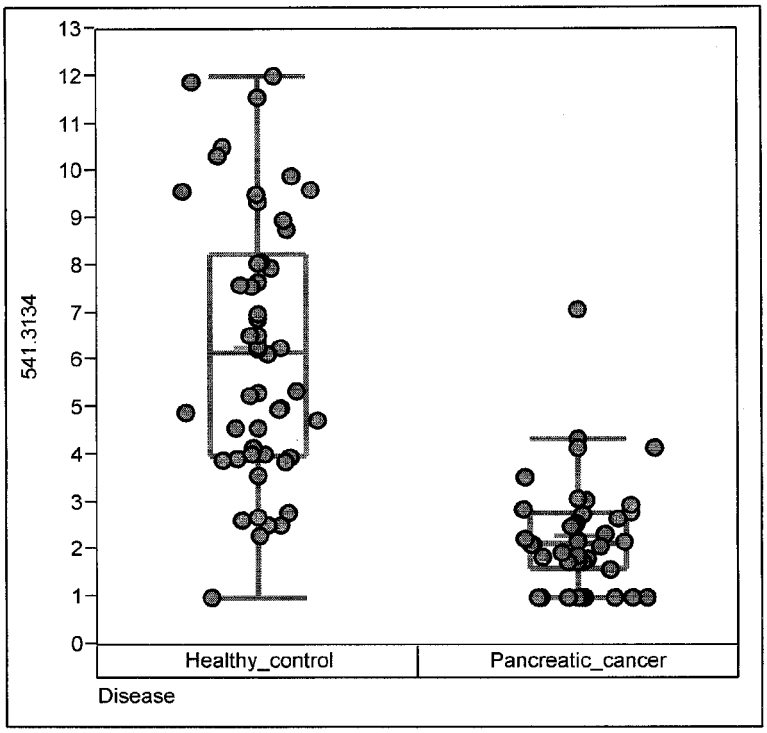


Figure 4 (cont.)

(f)



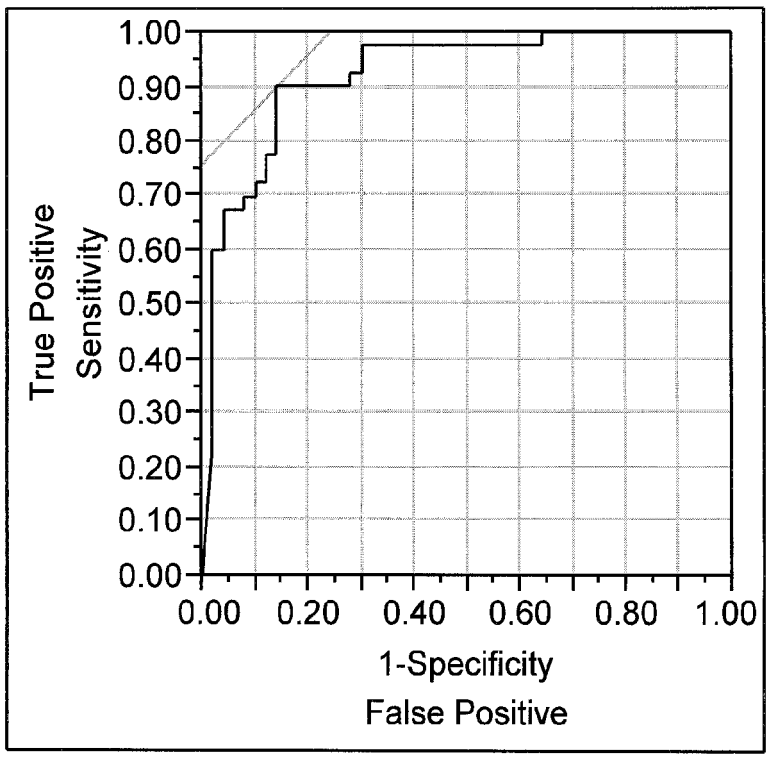
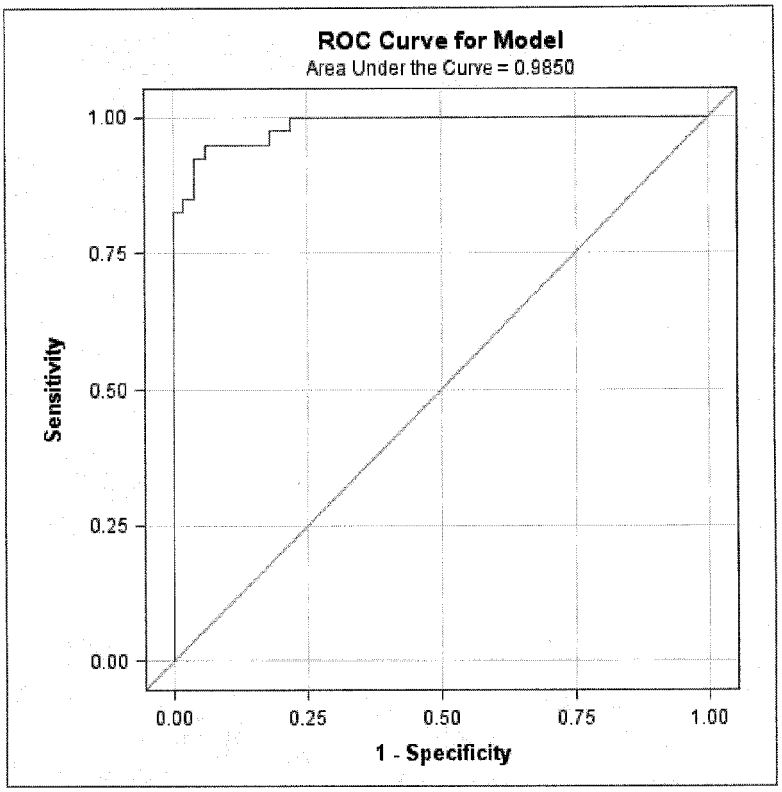


Figure 4 (cont.)

(a)



(b)

Classification Table									
Prob Level	Correct		Incorrect		Percentages				
	Event	Non-Event	Event	Non-Event	Correct	Sensi-tivity	Speci-ficity	FALSE	FALSE NEG
0.05	38	36	14	2	82.2	95	72	26.9	5.3
0.1	38	40	10	2	86.7	95	80	20.8	4.8
0.15	38	41	9	2	87.8	95	82	19.1	4.7
0.2	38	42	8	2	88.9	95	84	17.4	4.5
0.25	38	42	8	2	88.9	95	84	17.4	4.5
0.3	38	42	8	2	88.9	95	84	17.4	4.5
0.35	38	42	8	2	88.9	95	84	17.4	4.5
0.4	37	43	7	3	88.9	92.5	86	15.9	6.5
0.45	37	43	7	3	88.9	92.5	86	15.9	6.5
0.5	37	44	6	3	90	92.5	88	14	6.4
0.55	36	44	6	4	88.9	90	88	14.3	8.3
0.6	34	45	5	6	87.8	85	90	12.8	11.8
0.65	34	45	5	6	87.8	85	90	12.8	11.8
0.7	33	46	4	7	87.8	82.5	92	10.8	13.2
0.75	33	48	2	7	90	82.5	96	5.7	12.7
0.8	33	48	2	7	90	82.5	96	5.7	12.7
0.85	31	48	2	9	87.8	77.5	96	6.1	15.8
0.9	28	48	2	12	84.4	70	96	6.7	20
0.95	25	49	1	15	82.2	62.5	98	3.8	23.4
1	0	50	0	40	55.6	0	100	.	44.4

Figure 5

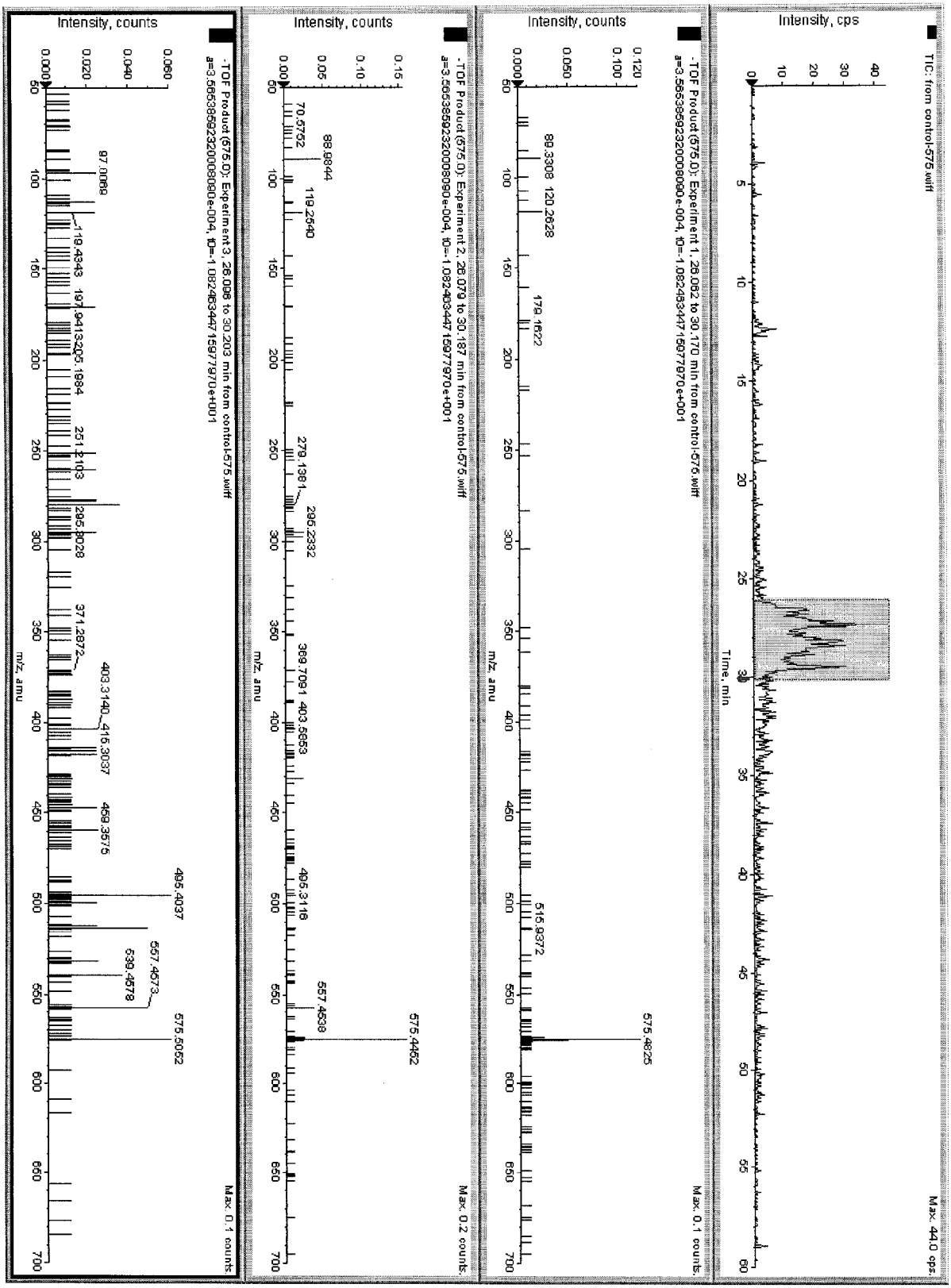

TIC: from control-575.wiff
Intensity, cps
Time, min
Max. 44.0 cps.
- TOF Product (575.0): Experiment 1, 28.062 to 30.170 min from control-575.wiff
a=3.56538592320008090e-004, t0=-1.08245344715977970e+001
Intensity, counts
m/z, amu
Max. 0.1 counts
89.3308
120.2628
179.1622
515.9372
575.4825
- TOF Product (575.0): Experiment 2, 28.079 to 30.187 min from control-575.wiff
a=3.56538592320008090e-004, t0=-1.08246344715977970e+001
Max. 0.2 counts
70.5752
88.9844
119.2540
279.1381
296.2392
369.7091
403.5653
495.3116
557.4538
575.4452
- TOF Product (575.0): Experiment 3, 28.096 to 30.203 min from control-575.wiff
a=3.56538592320008090e-004, t0=-1.08246344715977970e+001
Max. 0.1 counts
97.0069
119.4343
197.9413
205.1884
251.2103
295.8028
371.2872
403.3140
416.3037
459.3575
495.4037
557.4573
539.4578
575.5052

Figure 6

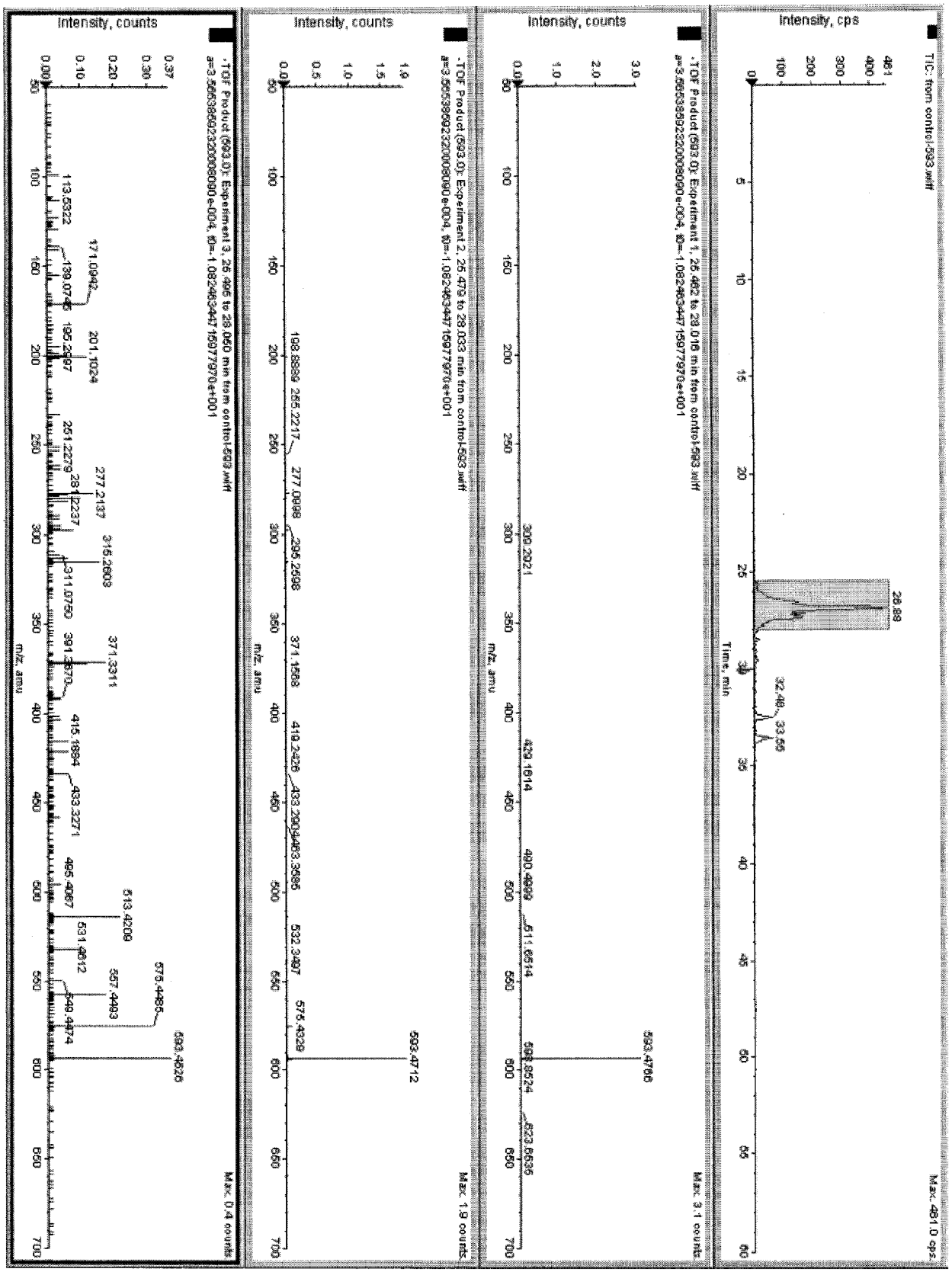

TIC: from control-593.wiff
Intensity, cps
Time, min
Max: 461.0 cps.
-TOF Product (593.0): Experiment 1, 26.462 to 29.016 min from control-593.wiff
Intensity, counts
m/z, amu
Max: 3.1 counts.
-TOF Product (593.0): Experiment 2, 25.479 to 28.033 min from control-593.wiff
Max: 1.9 counts.
-TOF Product (593.0): Experiment 3, 26.495 to 28.050 min from control-593.wiff
Max: 0.4 counts.

Figure 7

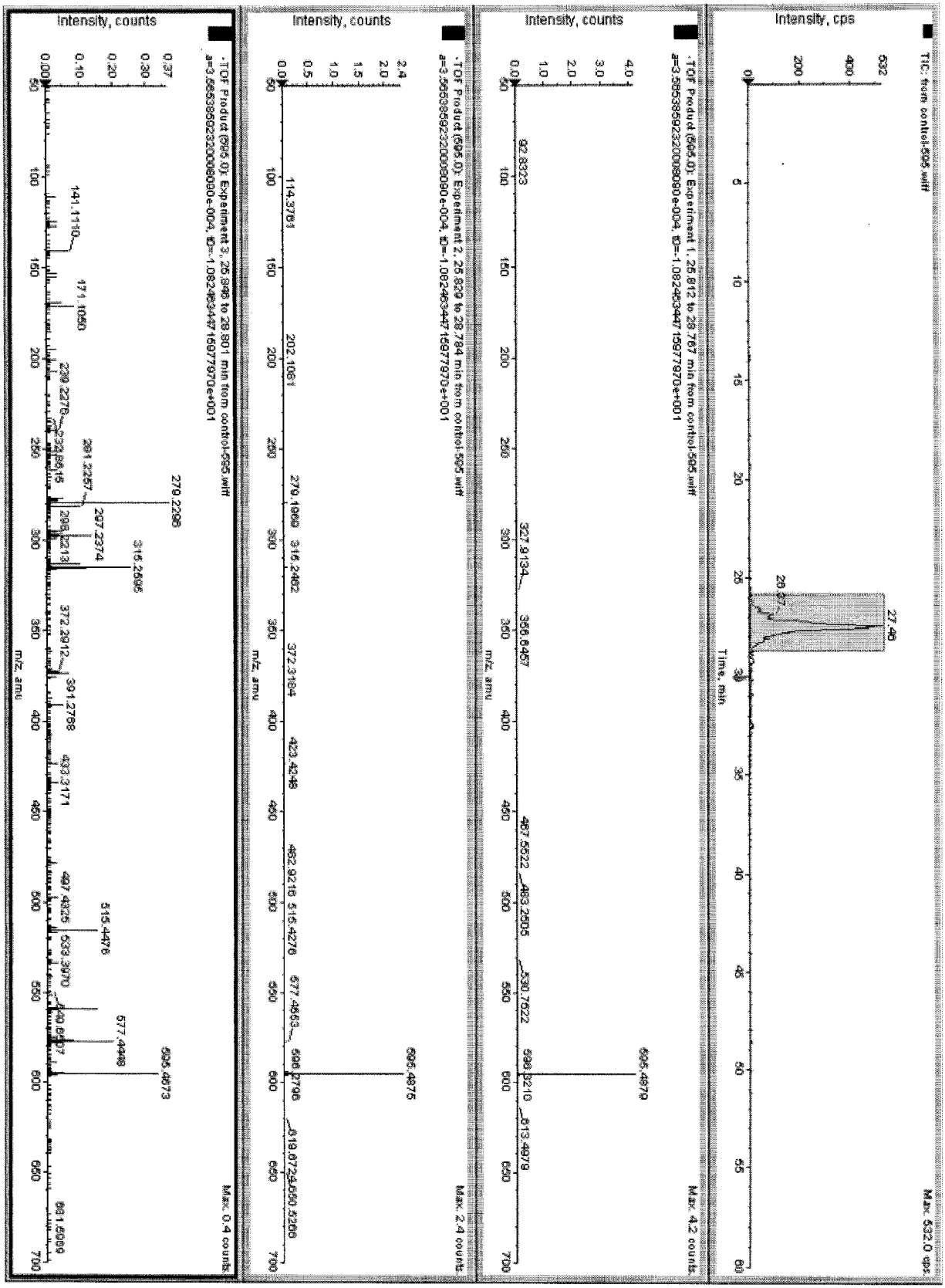

TIC: from control-595.wiff
Intensity, cps
Time, min
Max. 532.0 cps.
-TOF Product (595.0): Experiment 1, 26.612 to 28.767 min from control-595.wiff
Intensity, counts
m/z, amu
Max. 4.2 counts.
-TOF Product (595.0): Experiment 2, 25.829 to 28.784 min from control-595.wiff
Max. 2.4 counts.
-TOF Product (595.0): Experiment 3, 26.648 to 28.801 min from control-595.wiff
Max. 0.4 counts.

Figure 8

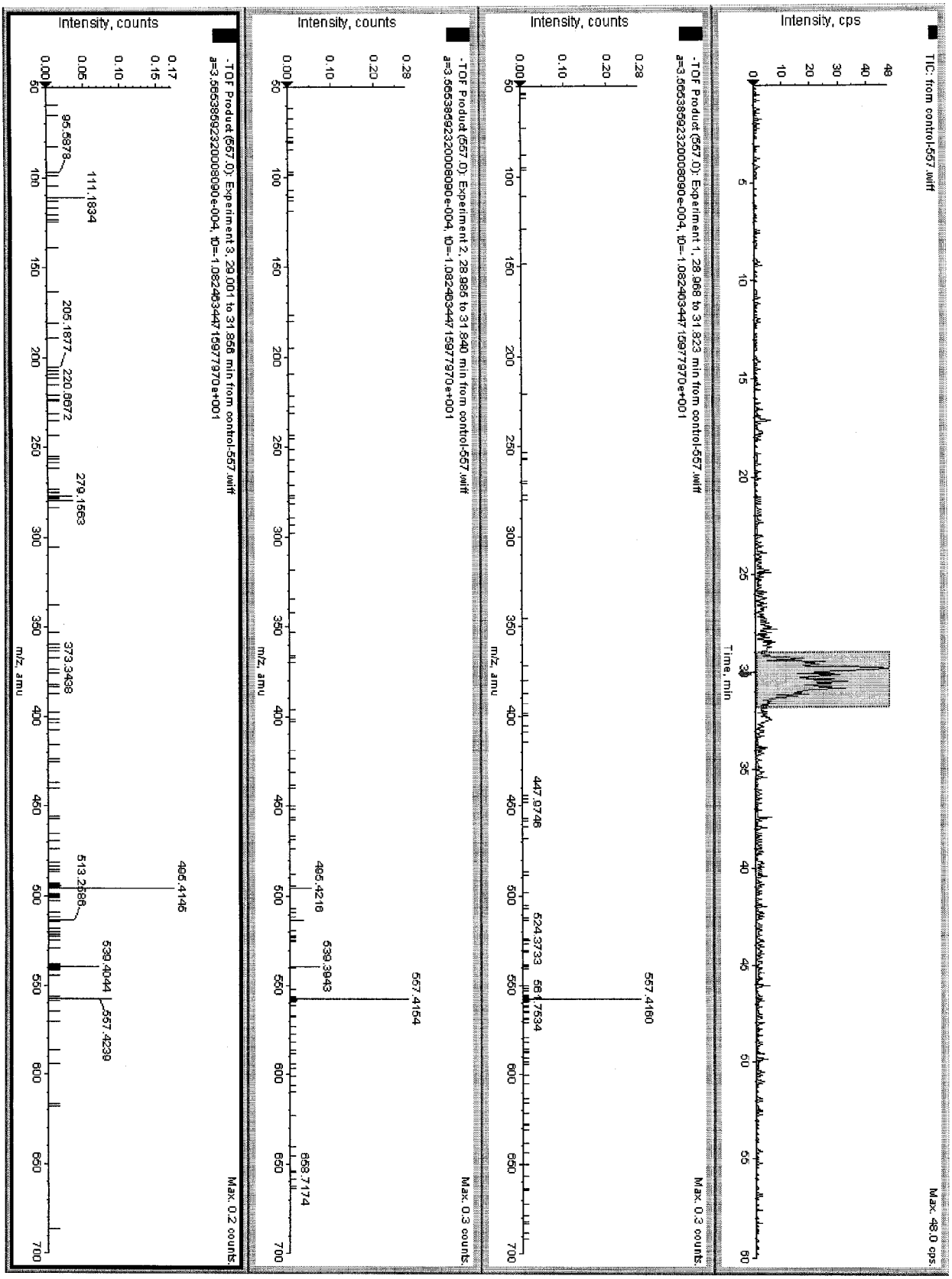

TIC: from control-557.wiff
Intensity, cps
Time, min
Max: 48.0 cps.
- TOF Product (557.0): Experiment 1, 28.968 to 31.823 min from control-557.wiff
a=3.56538592320008090e-004, t0=-1.08246344715977970e+001
Intensity, counts
m/z, amu
Max: 0.3 counts.
557.4160
447.9746
524.3733
581.7534
- TOF Product (557.0): Experiment 2, 28.985 to 31.840 min from control-557.wiff
557.4154
495.4216
539.3943
658.7174
- TOF Product (557.0): Experiment 3, 29.001 to 31.856 min from control-557.wiff
Max: 0.2 counts.
95.5878
111.1634
205.1677
220.6672
279.1563
373.3438
495.4146
513.2588
539.4044
557.4239

Figure 9

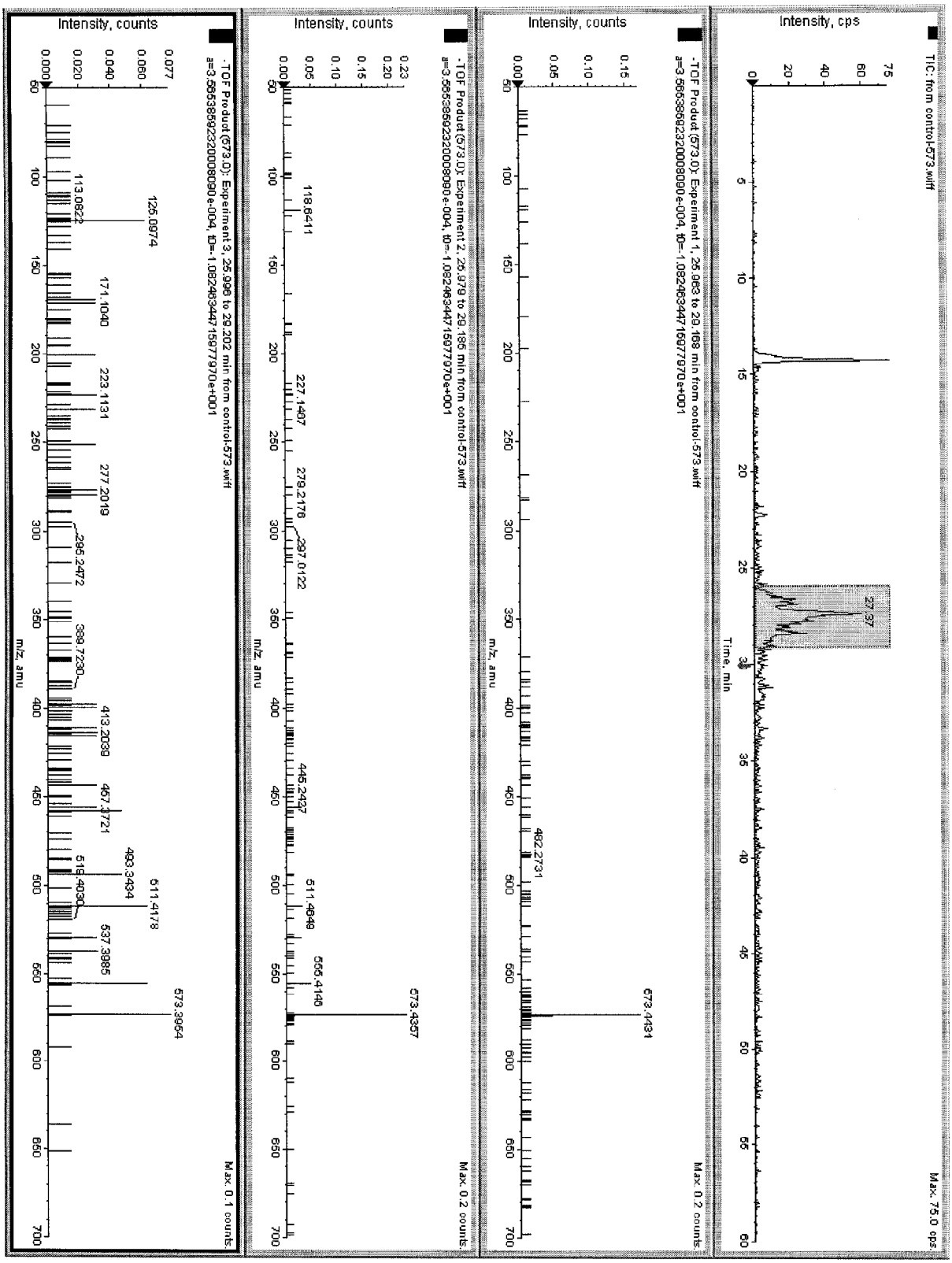

TIC: from control-573.wiff
Intensity, cps
Max. 75.0 cps.
Time, min
27.37
-TOF Product (573.0): Experiment 1, 25.963 to 29.168 min from control-573.wiff
a=3.66538692320008090e-004, t0=-1.08248344716977970e+001
Intensity, counts
Max. 0.2 counts.
m/z, amu
482.2731
573.4331
-TOF Product (573.0): Experiment 2, 25.979 to 29.185 min from control-573.wiff
a=3.66538692320008090e-004, t0=-1.08248344716977970e+001
Intensity, counts
Max. 0.2 counts.
m/z, amu
118.6411
227.1487
279.2178
297.0122
445.2427
511.4646
555.4146
573.4357
-TOF Product (573.0): Experiment 3, 26.996 to 29.202 min from control-573.wiff
a=3.66538692320008090e-004, t0=-1.08248344716977970e+001
Intensity, counts
Max. 0.1 counts.
m/z, amu
113.0822
125.0974
171.1040
223.1131
277.2019
295.2472
369.7230
413.2039
457.3721
493.3434
511.4178
519.4030
537.3985
573.3954

Figure 10

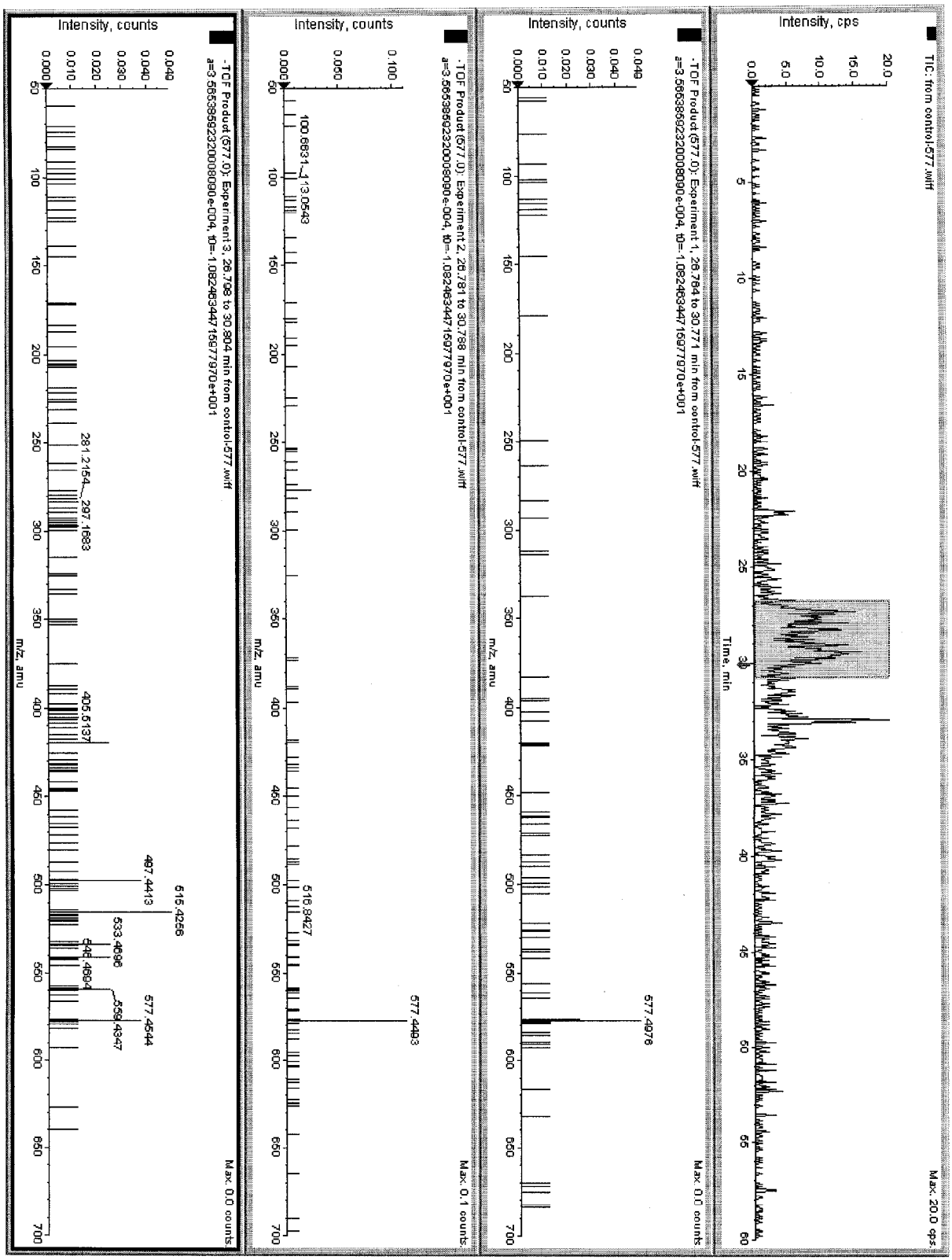

TIC: from control-577.wiff
Intensity, cps
Time, min
Max: 20.0 cps
-TOF Product (577.0): Experiment 1, 28.784 to 30.771 min from control-577.wiff
Intensity, counts
m/z, amu
577.4976
Max: 0.0 counts
-TOF Product (577.0): Experiment 2, 28.781 to 30.788 min from control-577.wiff
100.6631
113.0543
516.8427
577.4493
Max: 0.1 counts
-TOF Product (577.0): Experiment 3, 28.798 to 30.804 min from control-577.wiff
281.2154
297.1683
405.5137
497.4413
515.4256
533.4696
548.4694
559.4347
577.4544
Max: 0.0 counts

Figure 11

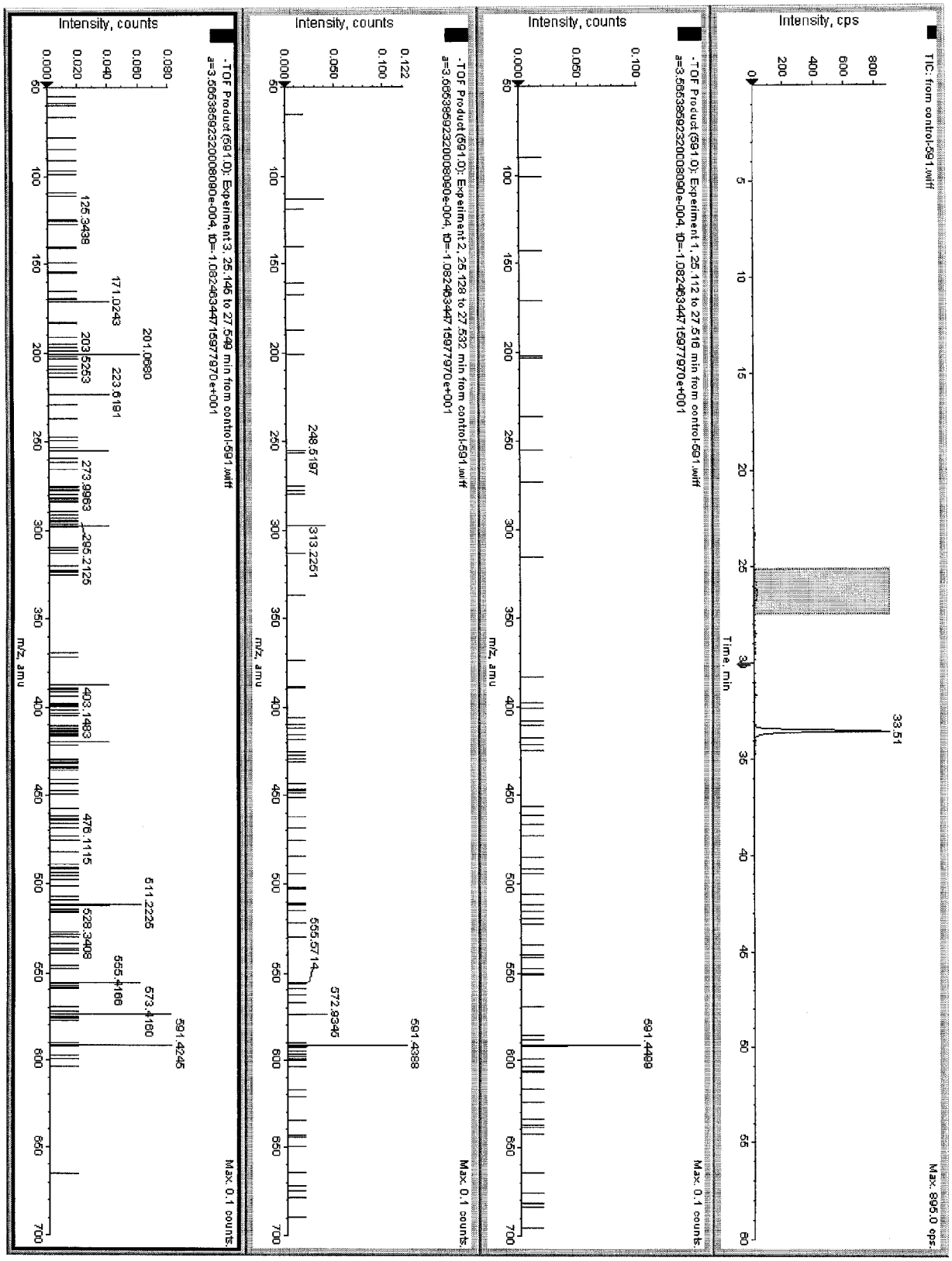

TIC: from control-591.wiff
Intensity, cps
Max. 895.0 cps.
33.51
Time, min
-TOF Product(591.0): Experiment 1, 25.112 to 27.516 min from control-591.wiff
a=3.56538592320080e-004, t0=-1.08246344715977970e+001
Intensity, counts
Max. 0.1 counts.
591.4489
m/z, amu
-TOF Product(591.0): Experiment 2, 25.128 to 27.532 min from control-591.wiff
a=3.56538592320080e-004, t0=-1.08246344715977970e+001
Intensity, counts
Max. 0.1 counts.
248.5187
313.2251
555.5714
572.9345
591.4388
m/z, amu
-TOF Product(591.0): Experiment 3, 25.145 to 27.549 min from control-591.wiff
a=3.56538592320080e-004, t0=-1.08246344715977970e+001
Intensity, counts
Max. 0.1 counts.
125.3438
171.0243
201.0690
203.5263
223.6191
273.9963
295.2125
403.1483
476.1115
511.2225
528.3408
555.4166
573.4160
591.4246
m/z, amu

Figure 12

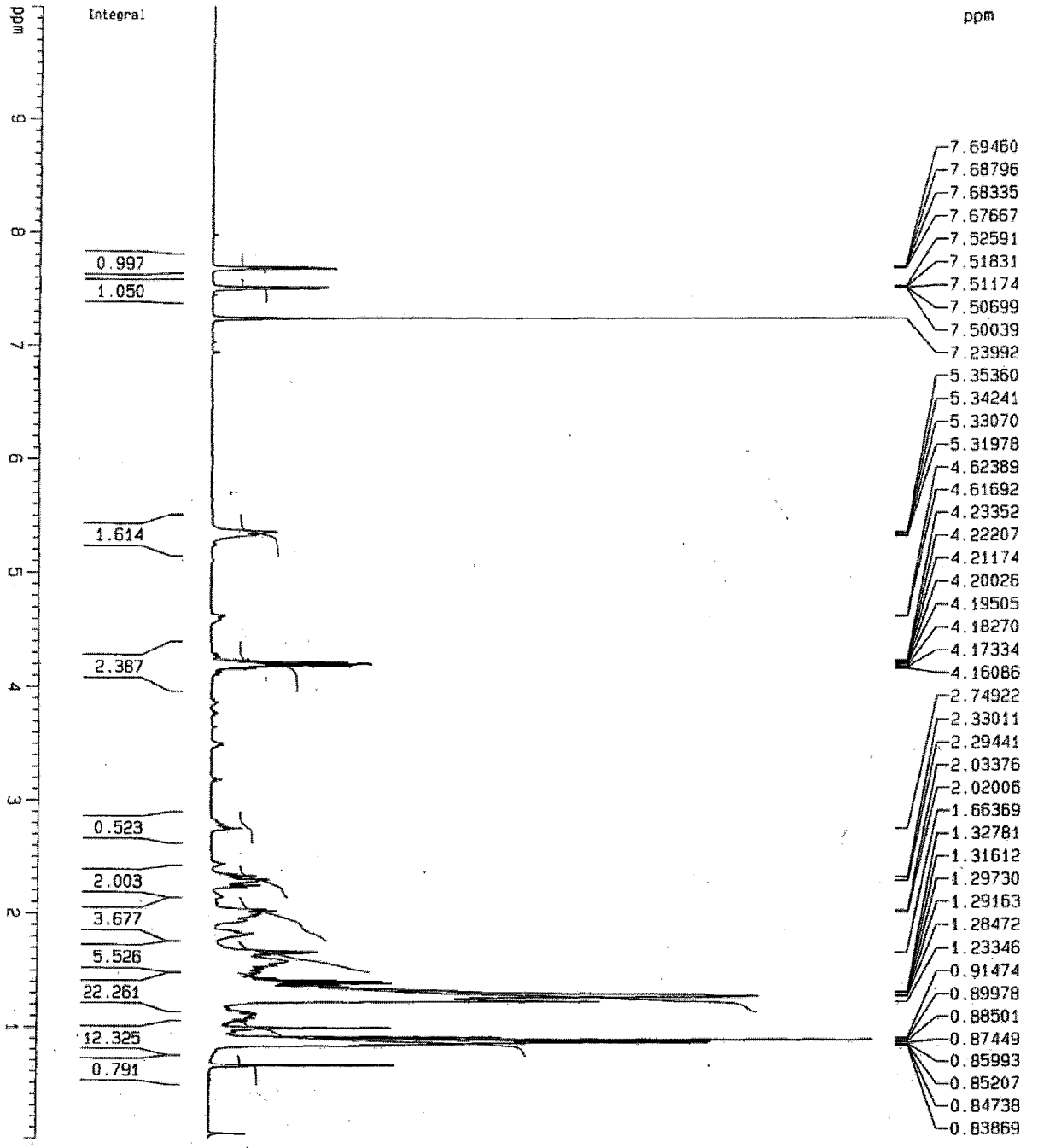

Integral
ppm
0.997
1.050
1.614
2.387
0.523
2.003
3.677
5.526
22.261
12.325
0.791
7.69460
7.68796
7.68335
7.67667
7.52591
7.51831
7.51174
7.50699
7.50039
7.23992
5.35360
5.34241
5.33070
5.31978
4.62389
4.61692
4.23352
4.22207
4.21174
4.20026
4.19505
4.18270
4.17334
4.16086
2.74922
2.33011
2.29441
2.03376
2.02006
1.66369
1.32781
1.31612
1.29730
1.29163
1.28472
1.23346
0.91474
0.89978
0.88501
0.87449
0.85993
0.85207
0.84738
0.83869

Figure 13

(a)

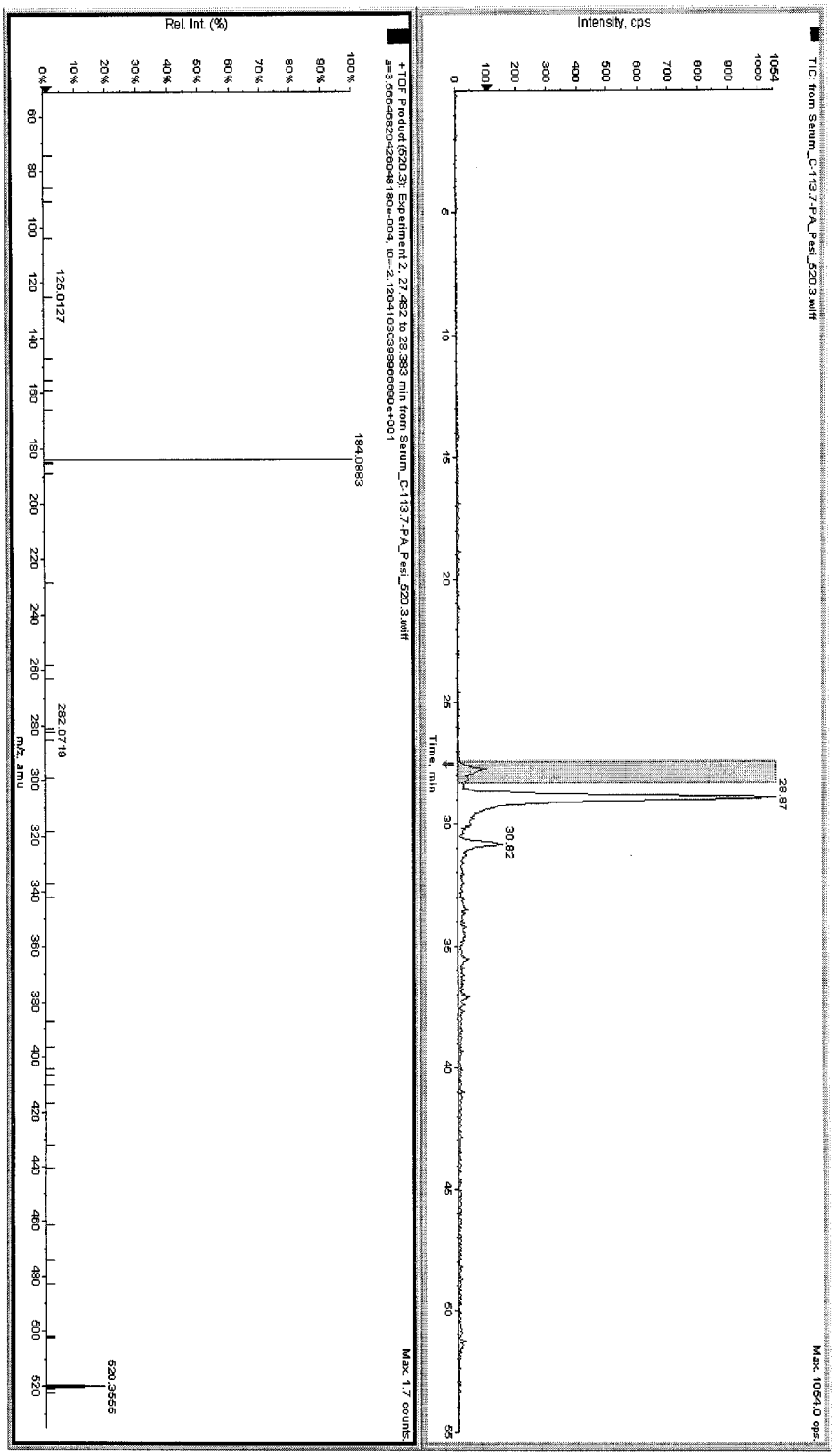

Rel. Int. (%)
Intensity, cps
Time, min
m/z, amu
125.0127
184.0883
282.0719
520.3555
28.87
30.82
Max. 1.7 counts.
Max. 1054.0 cps.

Figure 14

(b)

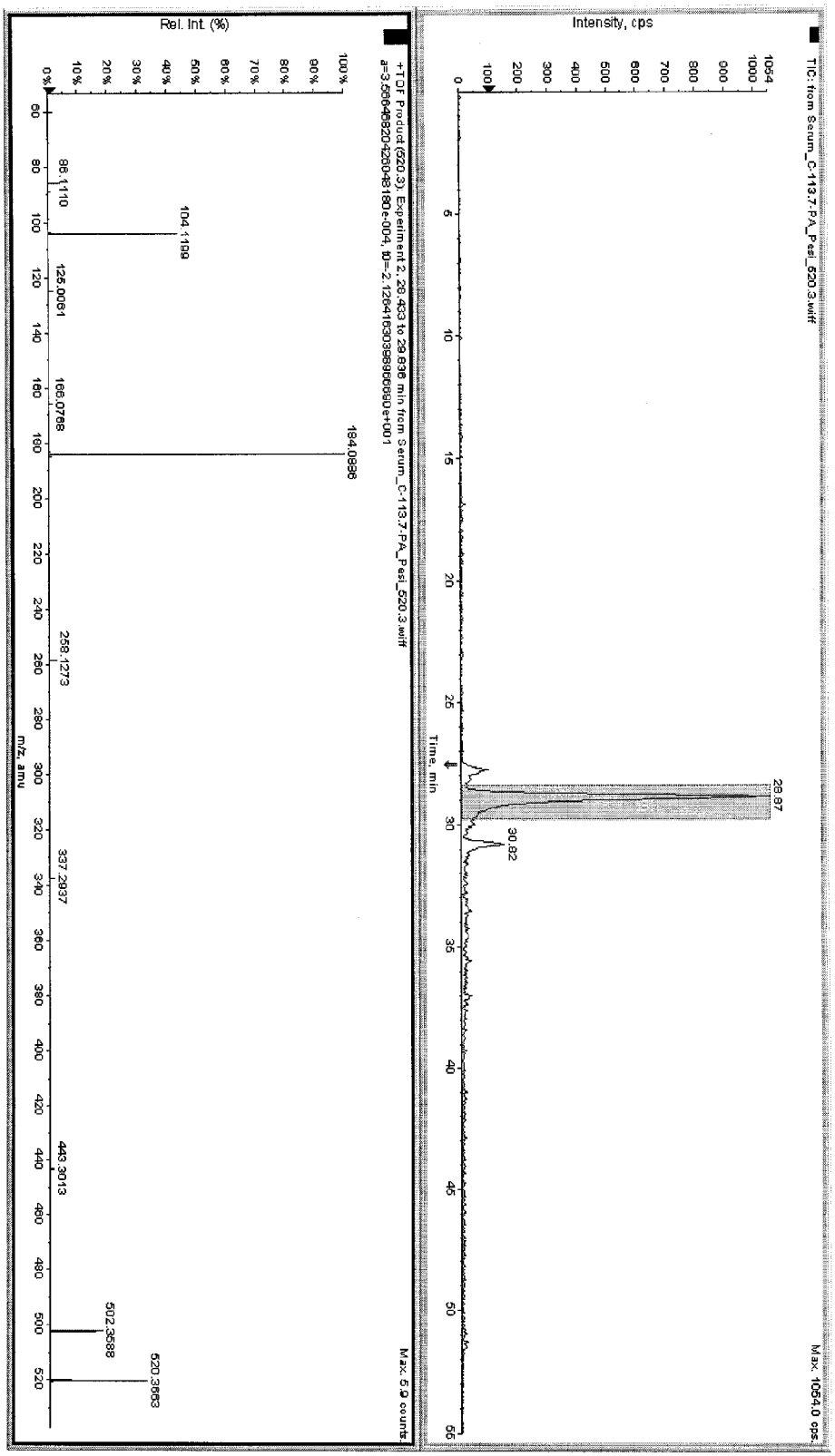


Figure 14 (cont.)

(a)

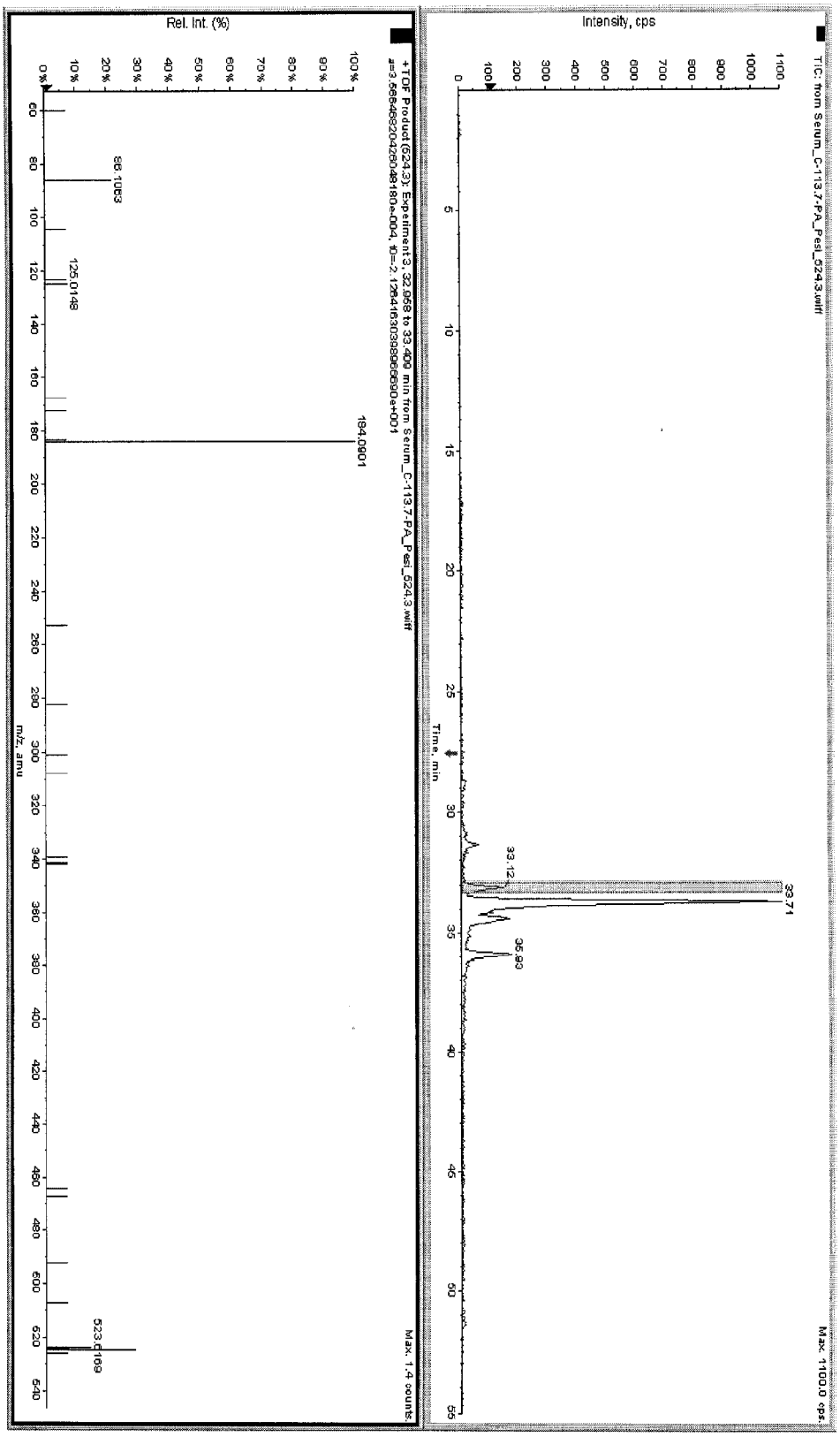

Rel. Int. (%)
+TOF Product(524.3): Experiment 3, 32.958 to 33.409 min from Serum_C-113.7-PA_Pesi_524.3.wiff
m/z, amu
86.1053
125.0148
184.0901
523.5169
Max. 1.4 counts
Intensity, cps
TIC: from Serum_C-113.7-PA_Pesi_524.3.wiff
Time, min
33.12
33.71
35.99
Max. 1100.0 cps.

Figure 15

(b)

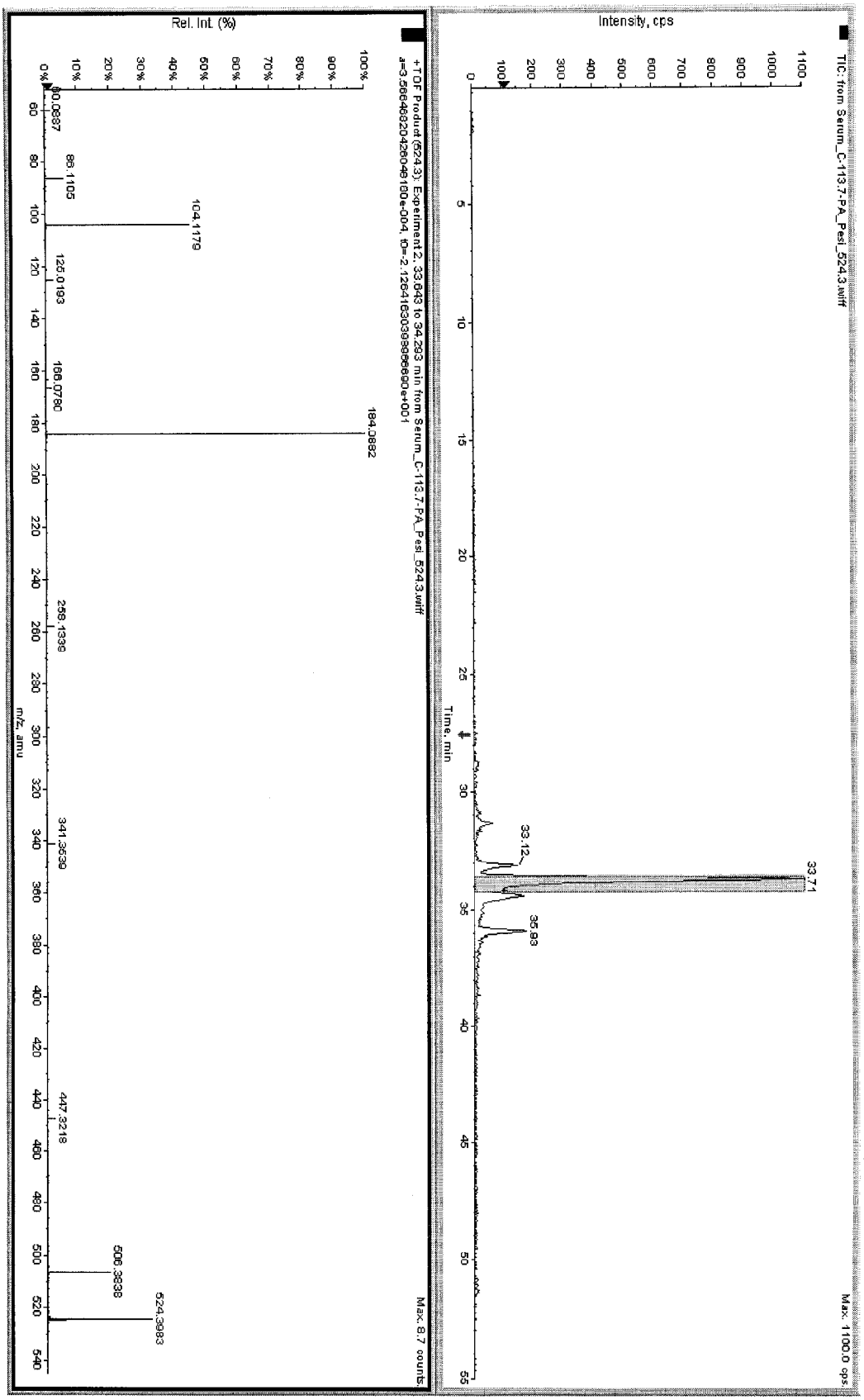


Figure 15 (cont.)

(a)

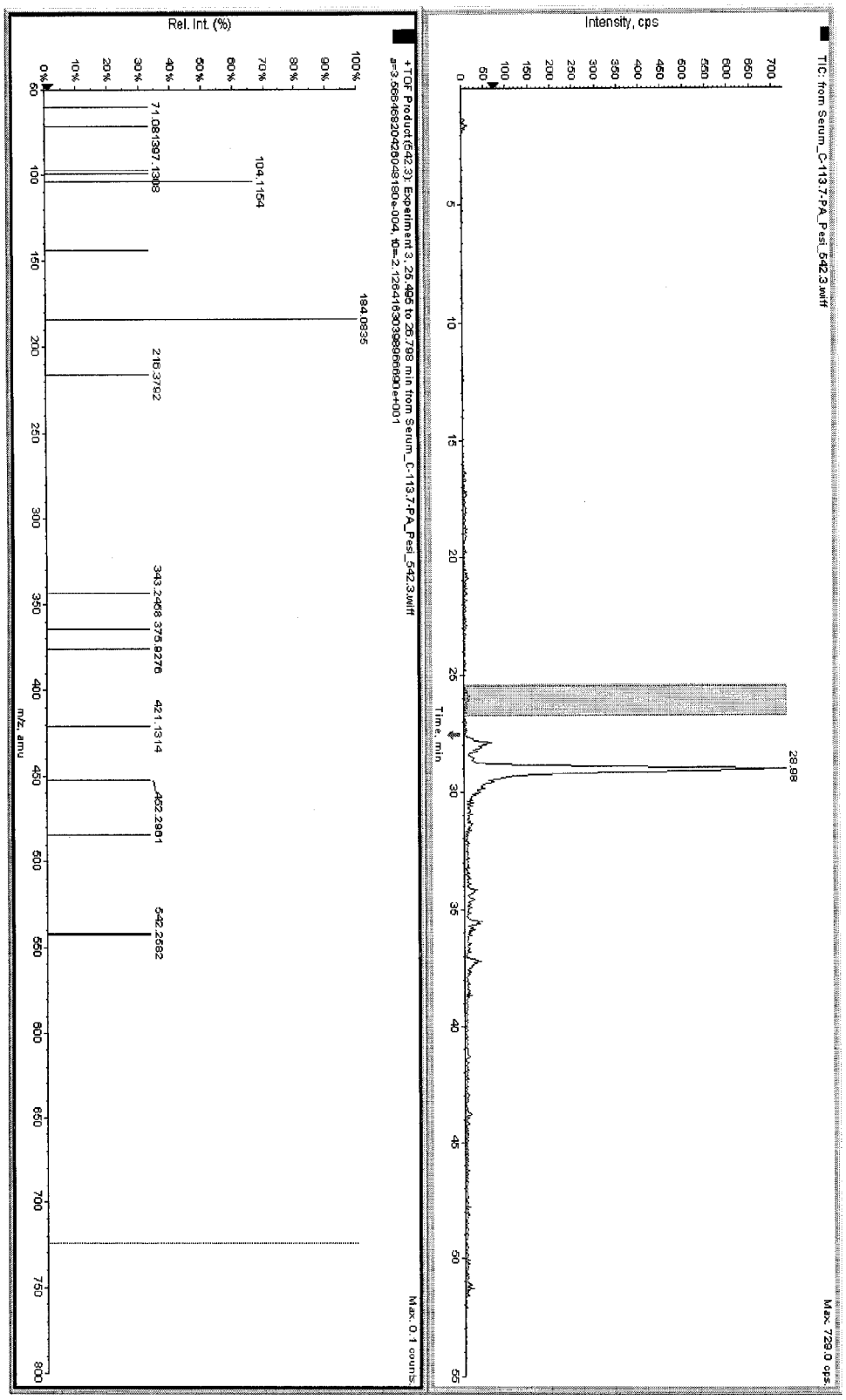

Rel. Int. (%)
m/z, amu
+TOF Product(542.3): Experiment 3, 25.425 to 26.799 min from Serum_C-113.7-PA_Pest_542.3.wiff
Max. 0.1 counts
71.0813
97.1308
104.1554
184.0835
216.3762
343.2468
375.5276
421.1314
452.2951
542.2682
Intensity, cps
Time, min
TIC: from Serum_C-113.7-PA_Pest_542.3.wiff
Max. 729.0 cps
28.98

Figure 16

(b)

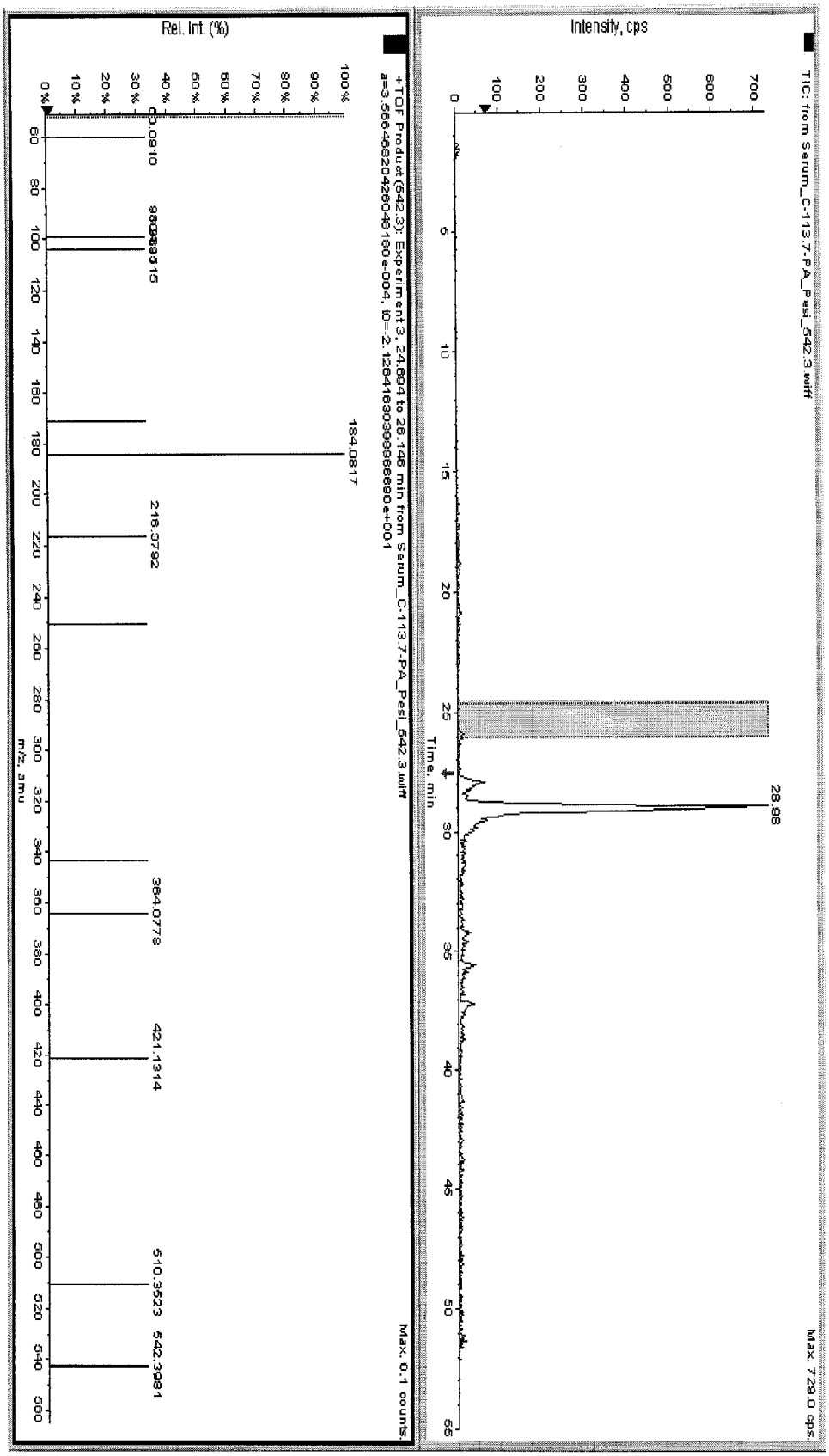


Figure 16 (cont.)

(c)

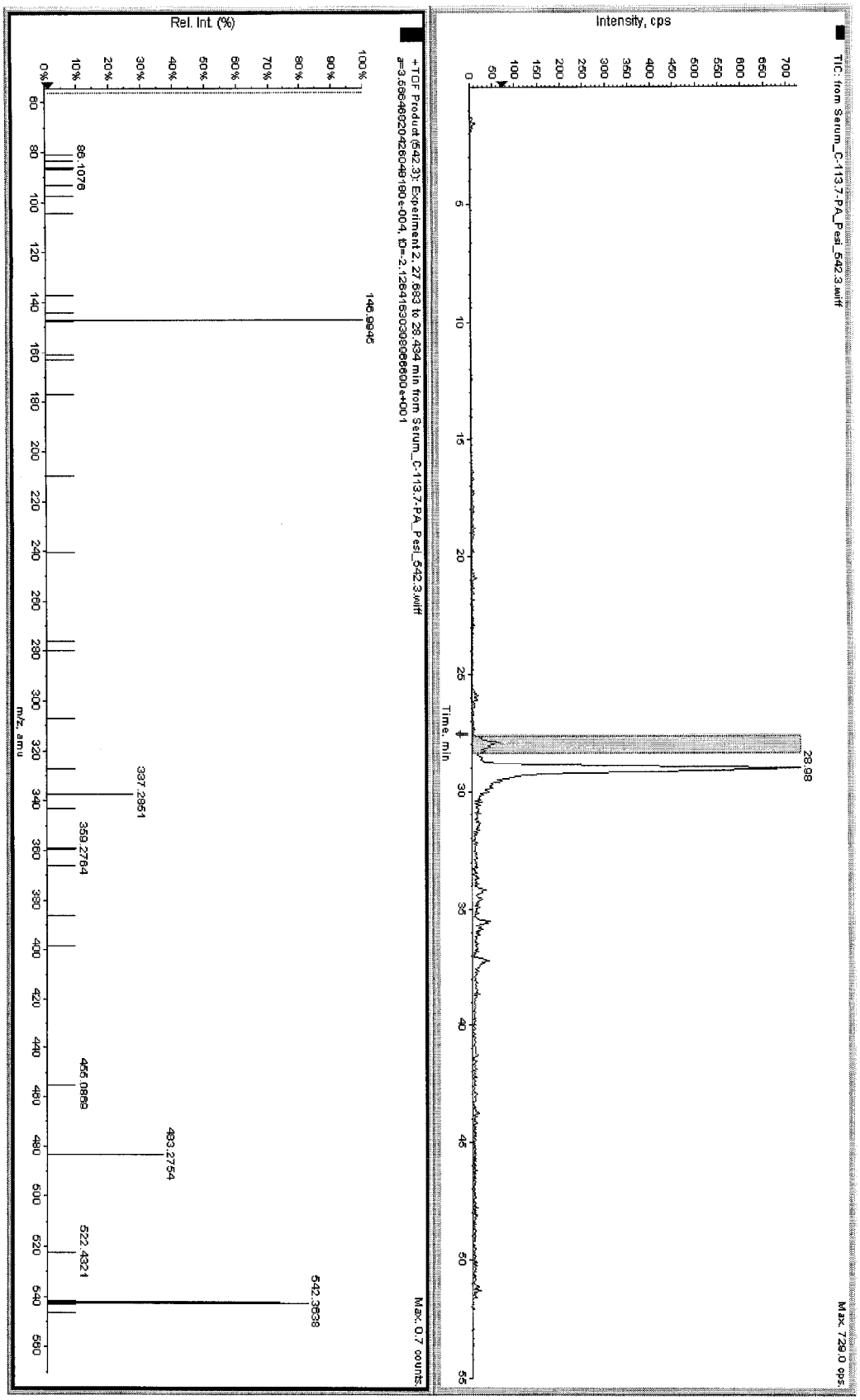


Figure 16 (cont.)

(d)

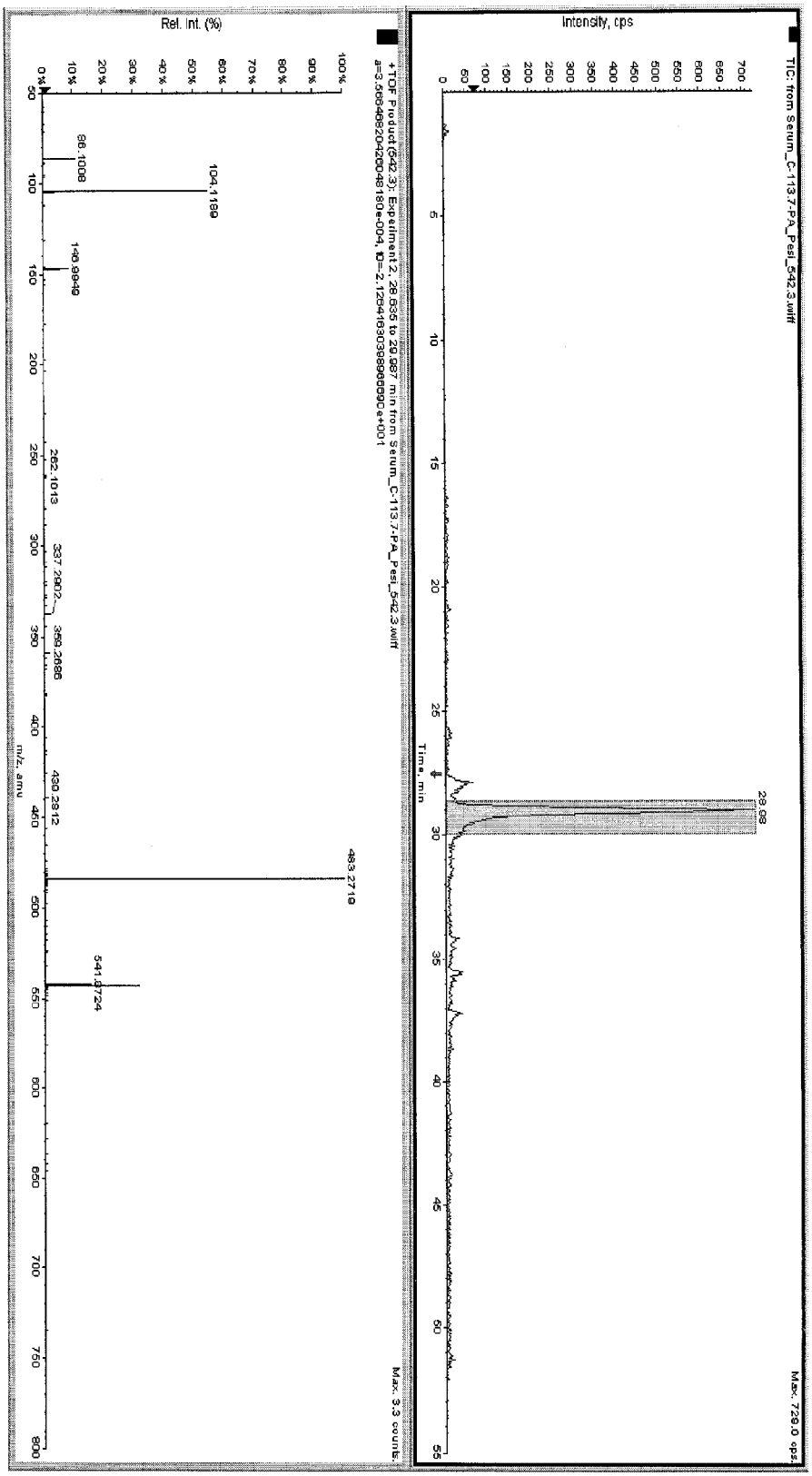


Figure 16 (cont.)

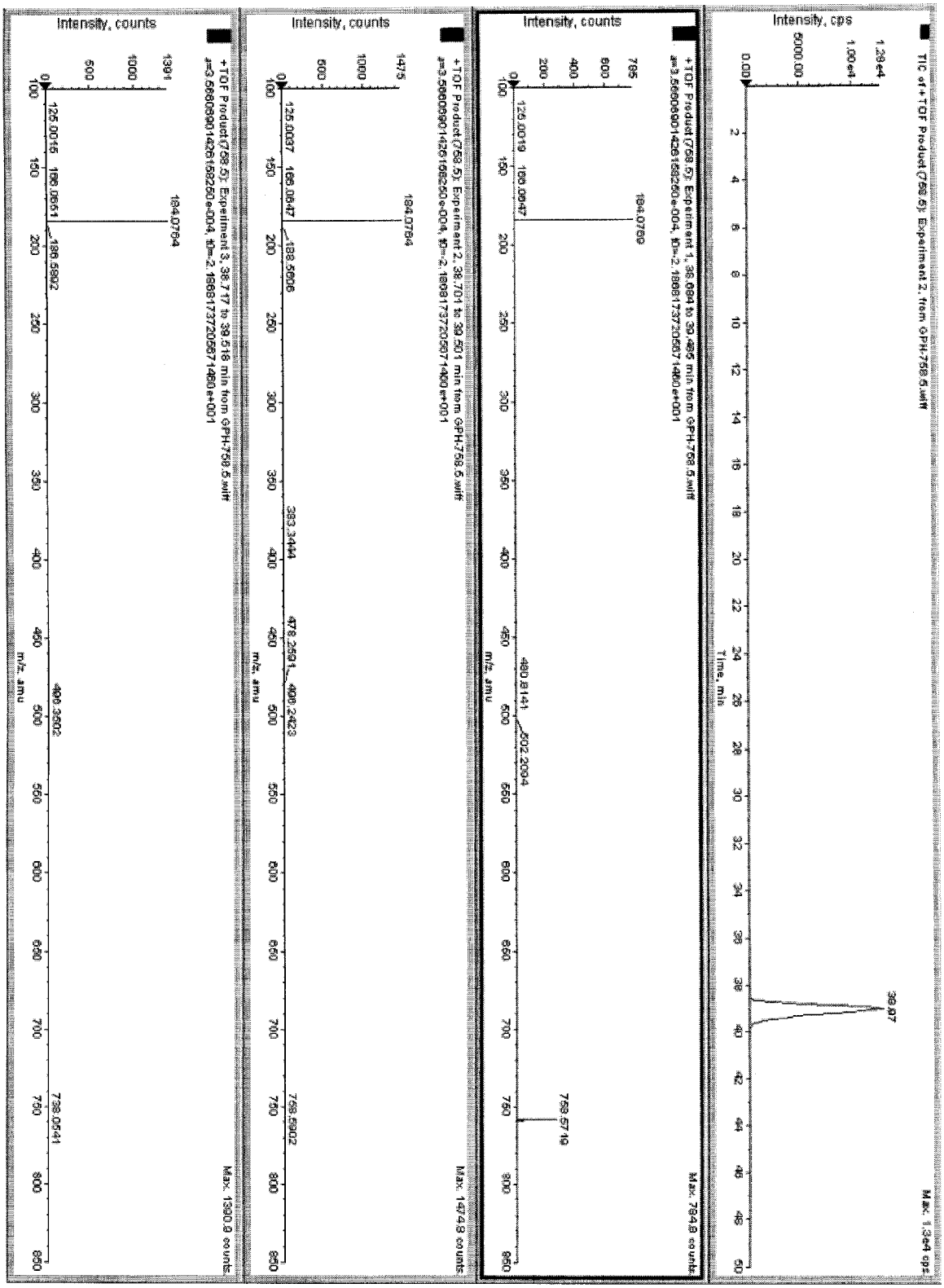

TIC of +TOF Product(758.5): Experiment 2, from GPH-758.5.wiff
Intensity, cps
Time, min
39.87
+TOF Product(758.5): Experiment 1, 36.694 to 39.485 min from GPH-758.5.wiff
Intensity, counts
m/z, amu
125.0019
186.0647
184.0769
480.8141
502.2004
758.5710
Max: 784.0 counts
+TOF Product(758.5): Experiment 2, 38.701 to 39.501 min from GPH-758.5.wiff
125.0037
186.0647
184.0784
188.5606
383.3444
478.2591
499.2423
758.5902
Max: 1474.0 counts
+TOF Product(758.5): Experiment 3, 38.717 to 39.518 min from GPH-758.5.wiff
125.0016
186.0661
184.0764
186.5892
499.3502
738.0541
Max: 1390.0 counts

Figure 17

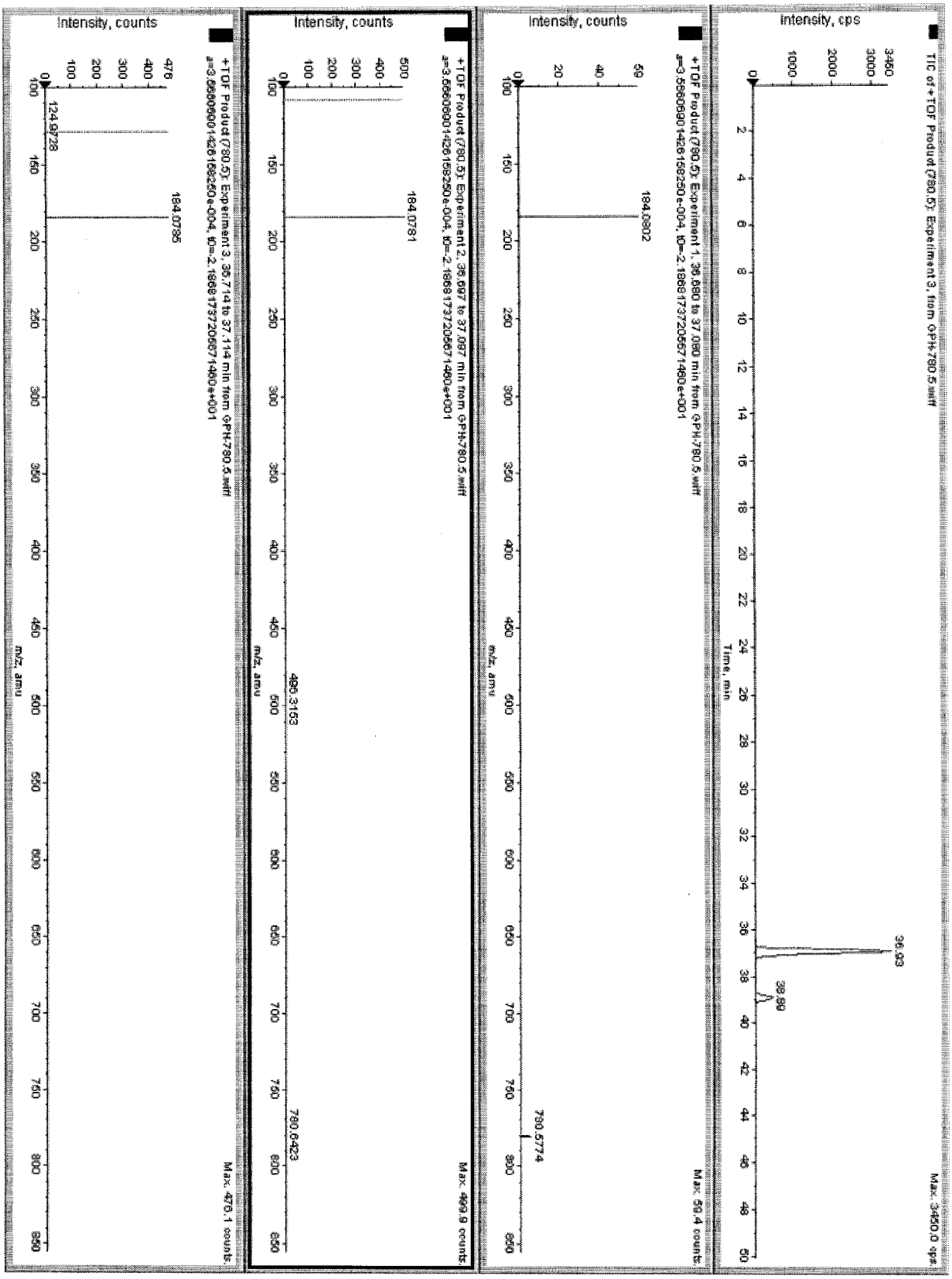

TIC of +TOF Product (780.5): Experiment 3, from GPH-780.5.wiff
Intensity, cps
Time, min
Max. 3450.0 cps.
36.93
39.89
+TOF Product (780.5): Experiment 1, 36.680 to 37.080 min from GPH-780.5.wiff
Intensity, counts
m/z, amu
Max. 59.4 counts.
184.0802
780.5774
+TOF Product (780.5): Experiment 2, 36.697 to 37.097 min from GPH-780.5.wiff
Intensity, counts
m/z, amu
Max. 499.9 counts.
184.0781
486.3153
780.6423
+TOF Product (780.5): Experiment 3, 36.714 to 37.114 min from GPH-780.5.wiff
Intensity, counts
m/z, amu
Max. 476.1 counts.
184.0795
124.9728

Figure 18

(a)

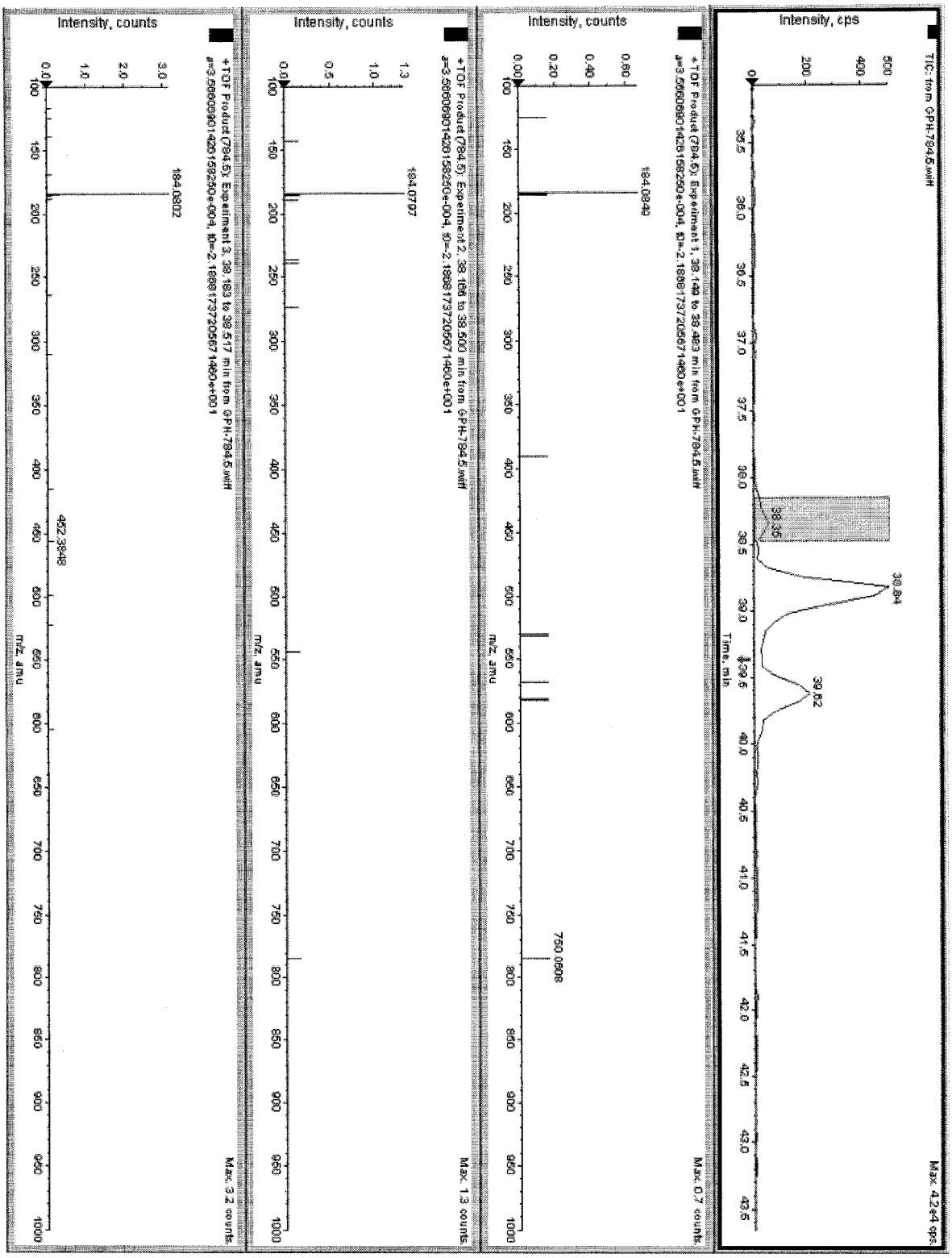

TIC: from GPH-7845.wiff
Intensity, eps
Max. 4.2e+4 cps.
38.36
38.84
39.52
Time, min
+TOF Product (784.5): Experiment 1, 38.140 to 38.483 min from GPH-7845.wiff
Intensity, counts
184.0840
750.0508
Max. 0.7 counts.
+TOF Product (784.5): Experiment 2, 38.168 to 38.500 min from GPH-7845.wiff
184.0797
Max. 1.3 counts.
+TOF Product (784.5): Experiment 3, 38.183 to 38.517 min from GPH-7845.wiff
184.0802
462.3848
Max. 3.2 counts.
m/z, amu

Figure 19

(b)

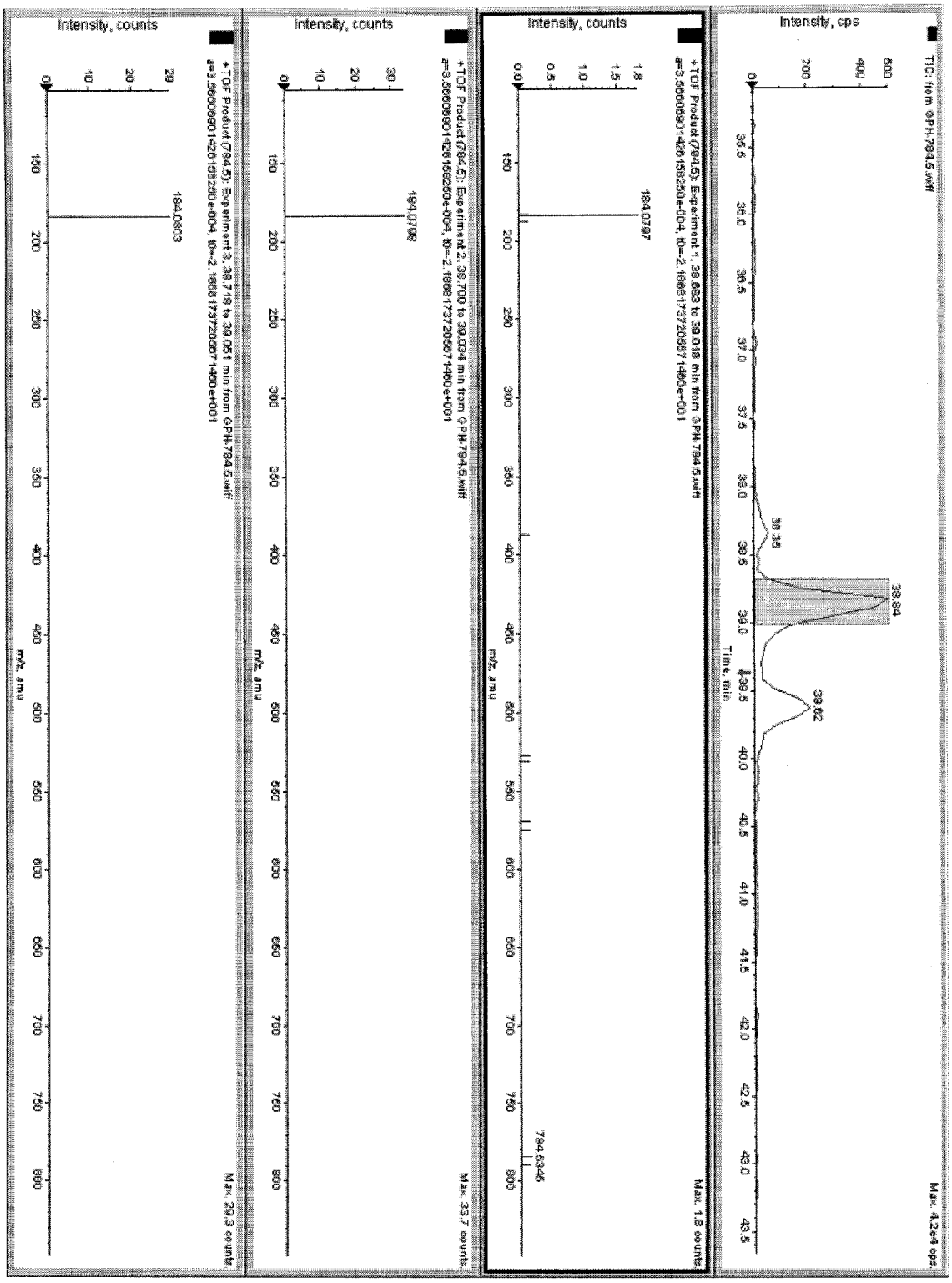


Figure 19 (Cont.)

(c)

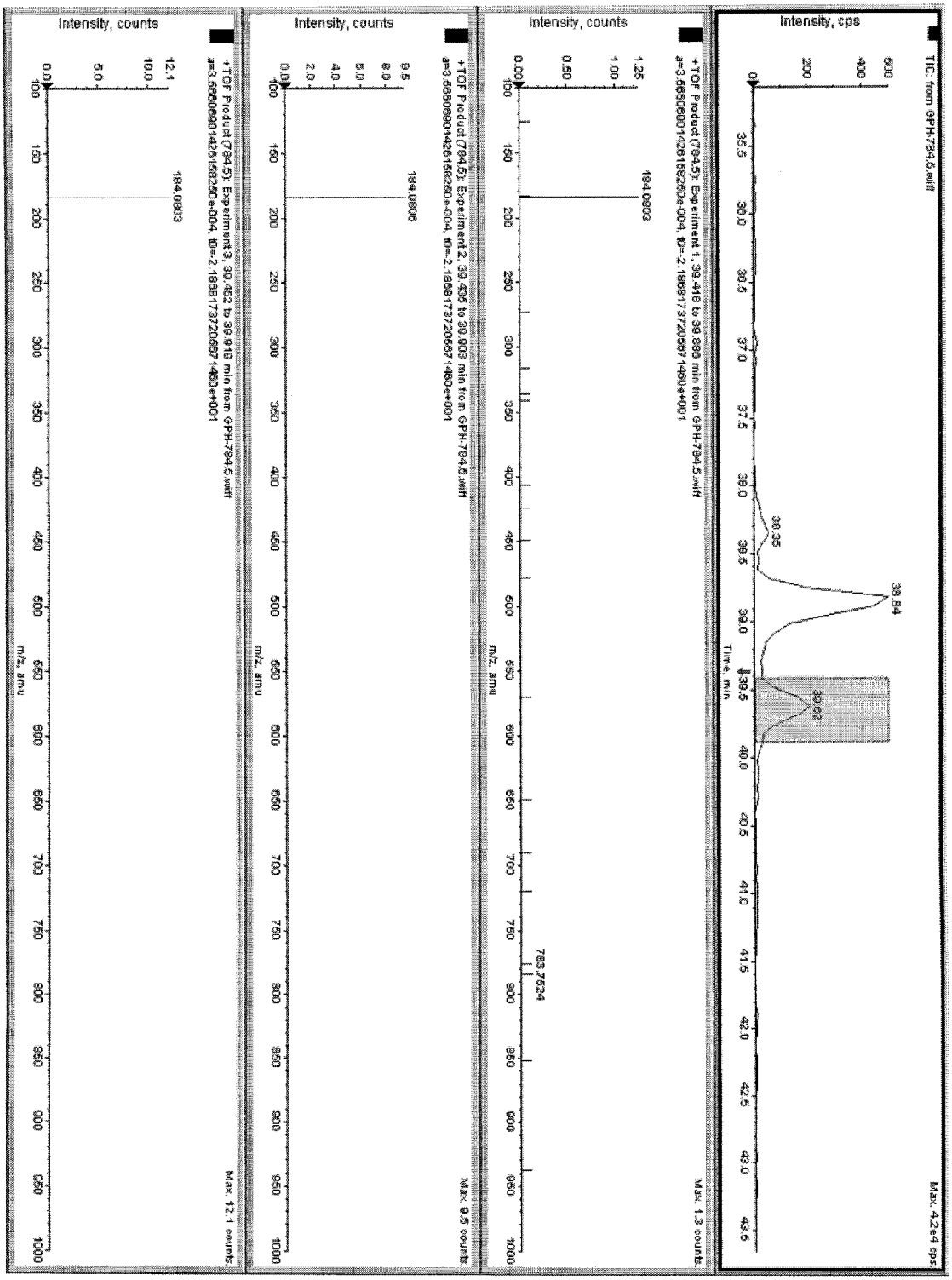


Figure 19 (Cont.)

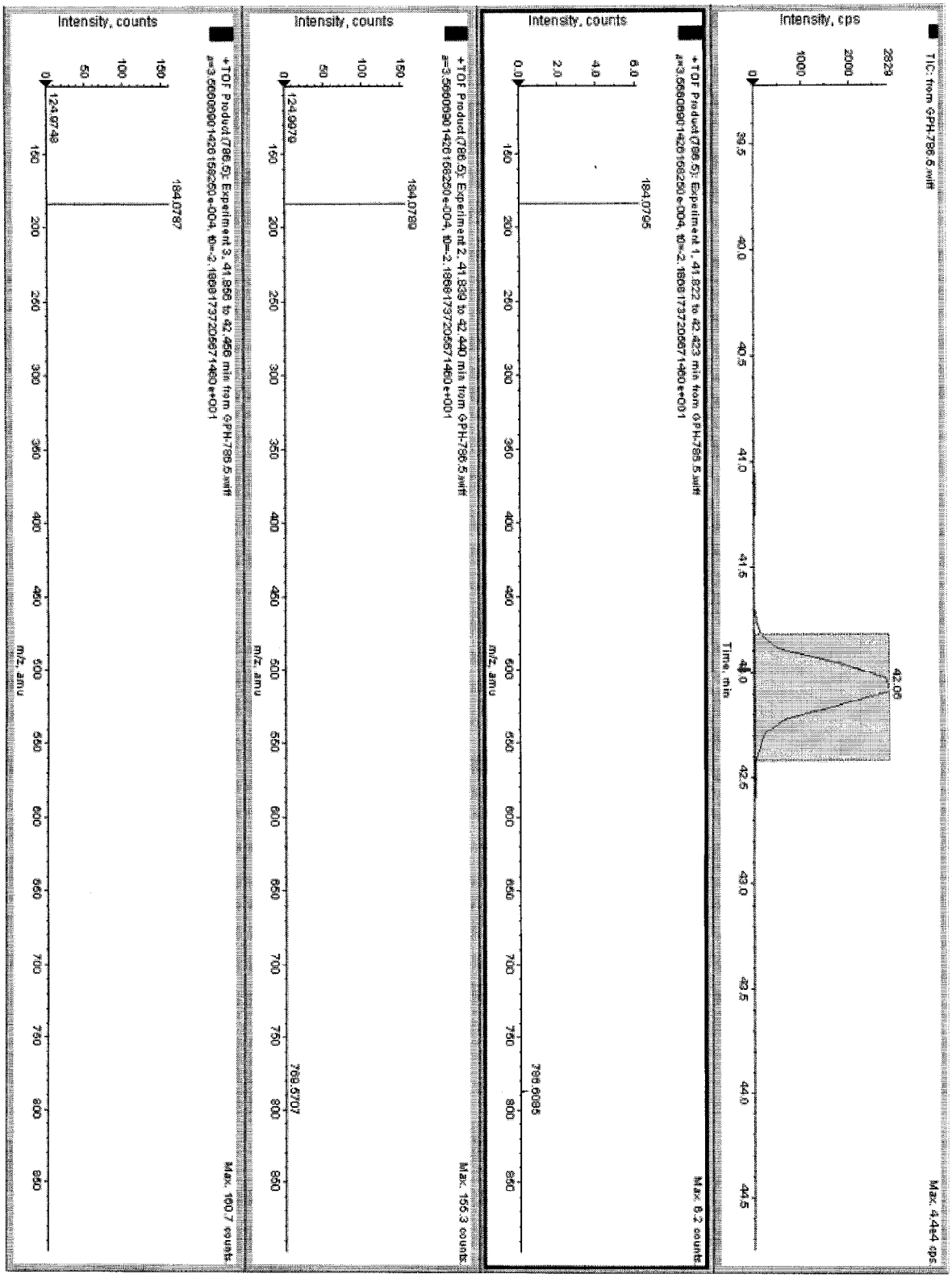

TIC: from GPH-786.5.wiff
Intensity, cps
Time, min
42.06
Max: 4.4e4 cps.
+TOF Product(786.5): Experiment 1, 41.822 to 42.423 min from GPH-786.5.wiff
Intensity, counts
m/z, amu
184.0795
786.6085
Max: 8.2 counts.
+TOF Product(786.5): Experiment 2, 41.839 to 42.440 min from GPH-786.5.wiff
Intensity, counts
m/z, amu
184.0789
769.5707
Max: 155.3 counts.
+TOF Product(786.5): Experiment 3, 41.856 to 42.456 min from GPH-786.5.wiff
Intensity, counts
m/z, amu
184.0787
124.9748
Max: 160.7 counts.

Figure 20

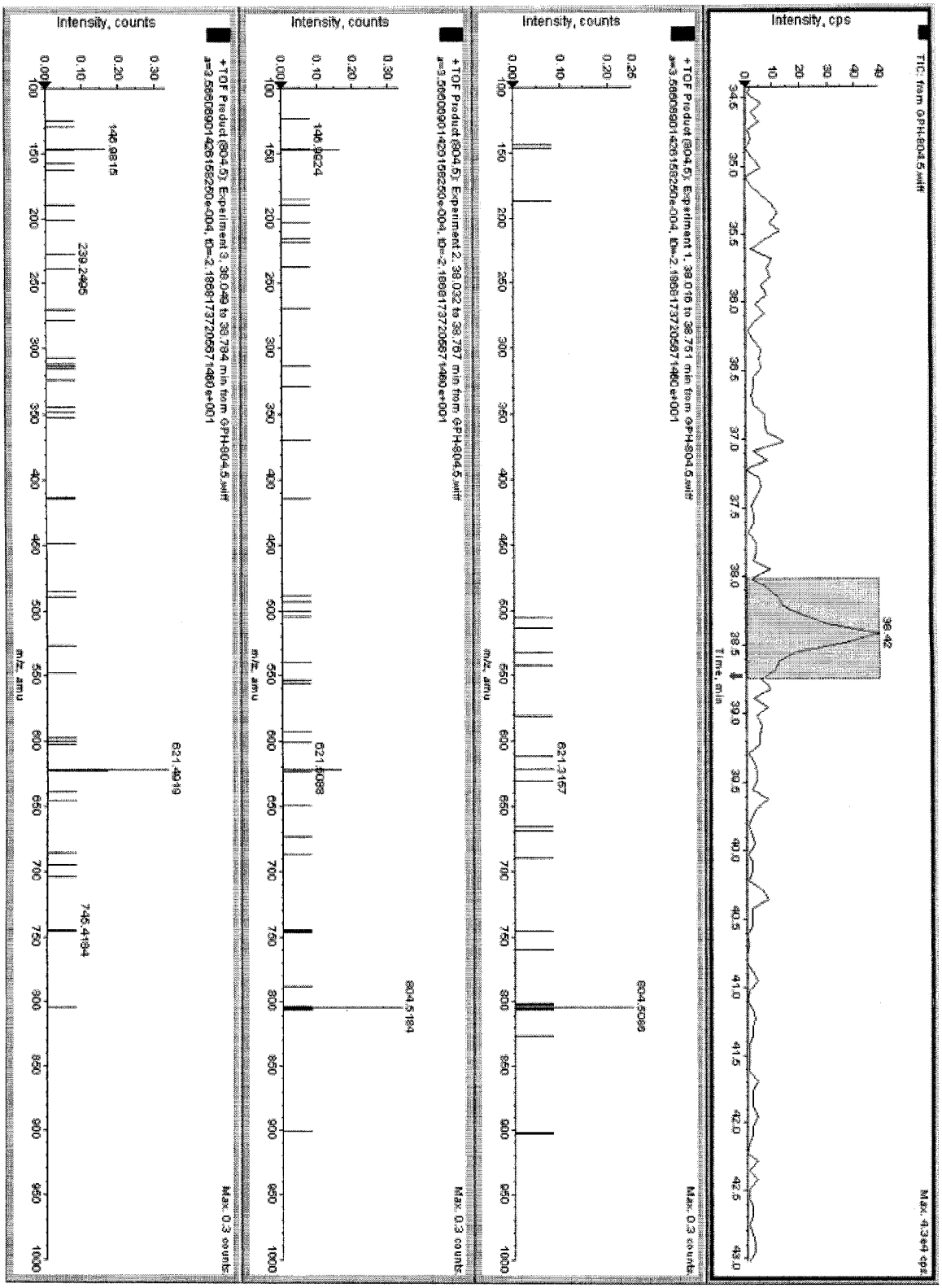

Intensity, cps
Time, min
38.42
Intensity, counts
m/z, amu
804.5099
621.3157
804.5184
621.3083
745.4184
621.4019
239.2405
148.9815
148.9824

Figure 21

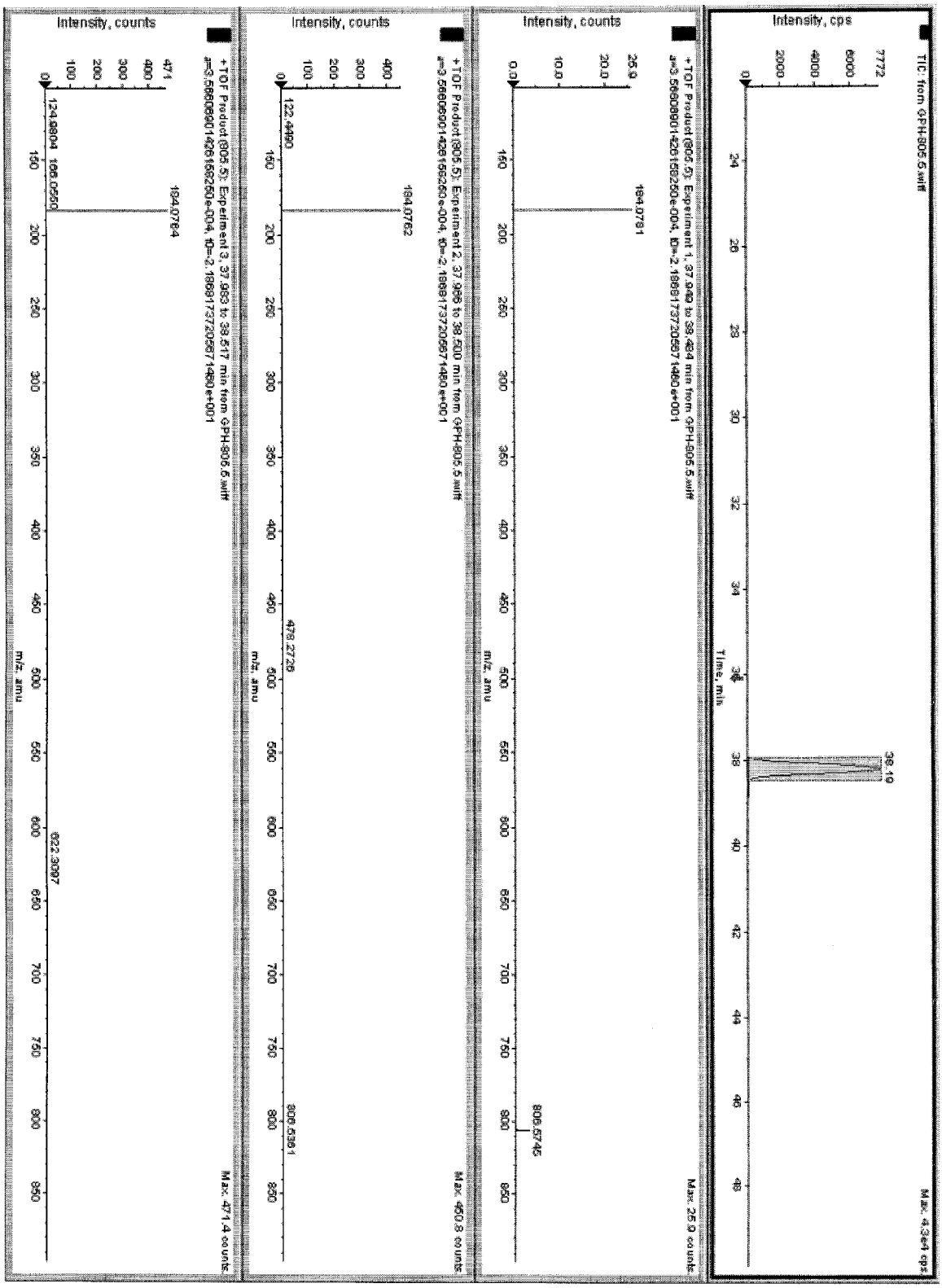

TIC from GPH-805.5.wiff
Intensity, cps
Time, min
38.19
Max. 4.3e4 cps
+TOF Product (805.5): Experiment 1, 37.940 to 39.484 min from GPH-805.5.wiff
Intensity, counts
184.0781
808.5745
m/z, amu
Max. 25.9 counts
+TOF Product (805.5): Experiment 2, 37.956 to 39.500 min from GPH-805.5.wiff
Intensity, counts
184.0762
478.2729
808.5361
m/z, amu
Max. 450.8 counts
+TOF Product (805.5): Experiment 3, 37.983 to 38.517 min from GPH-805.5.wiff
Intensity, counts
184.0784
124.9894
166.0550
922.3097
m/z, amu
Max. 471.4 counts

Figure 22

(a)

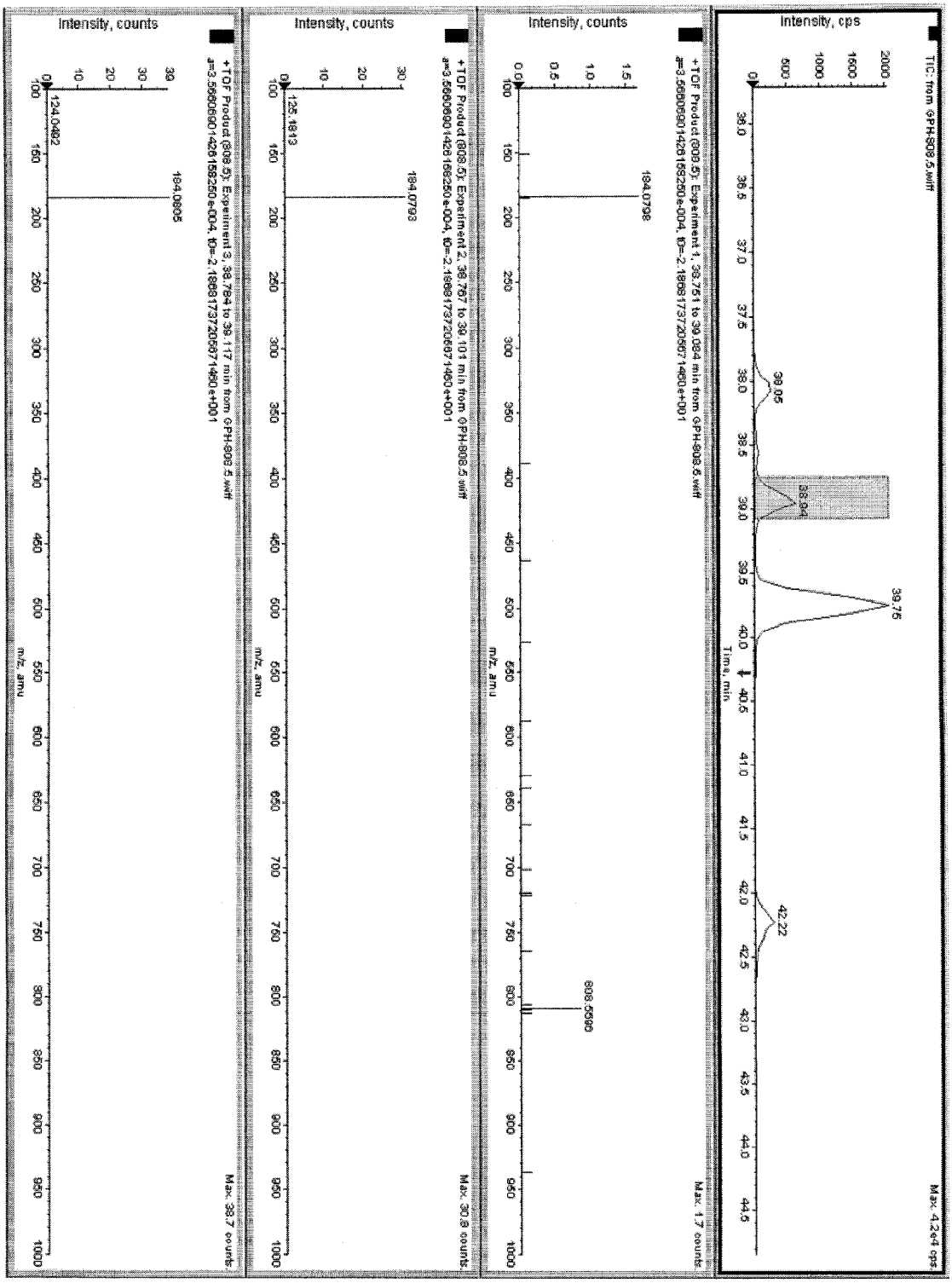

Intensity, cps
TIC: from GPH-808.5.wiff
Max: 4.2e+4 cps
38.05
38.94
39.75
42.22
Time, min
Intensity, counts
+TOF Product (808.5): Experiment 1, 38.751 to 39.084 min from GPH-808.5.wiff
Max: 1.7 counts
184.0798
808.5598
m/z, amu
Intensity, counts
+TOF Product (808.5): Experiment 2, 38.767 to 39.101 min from GPH-808.5.wiff
Max: 30.8 counts
184.0793
125.1813
m/z, amu
Intensity, counts
+TOF Product (808.5): Experiment 3, 38.784 to 39.117 min from GPH-808.5.wiff
Max: 38.7 counts
184.0805
124.0492
m/z, amu

Figure 23

(b)

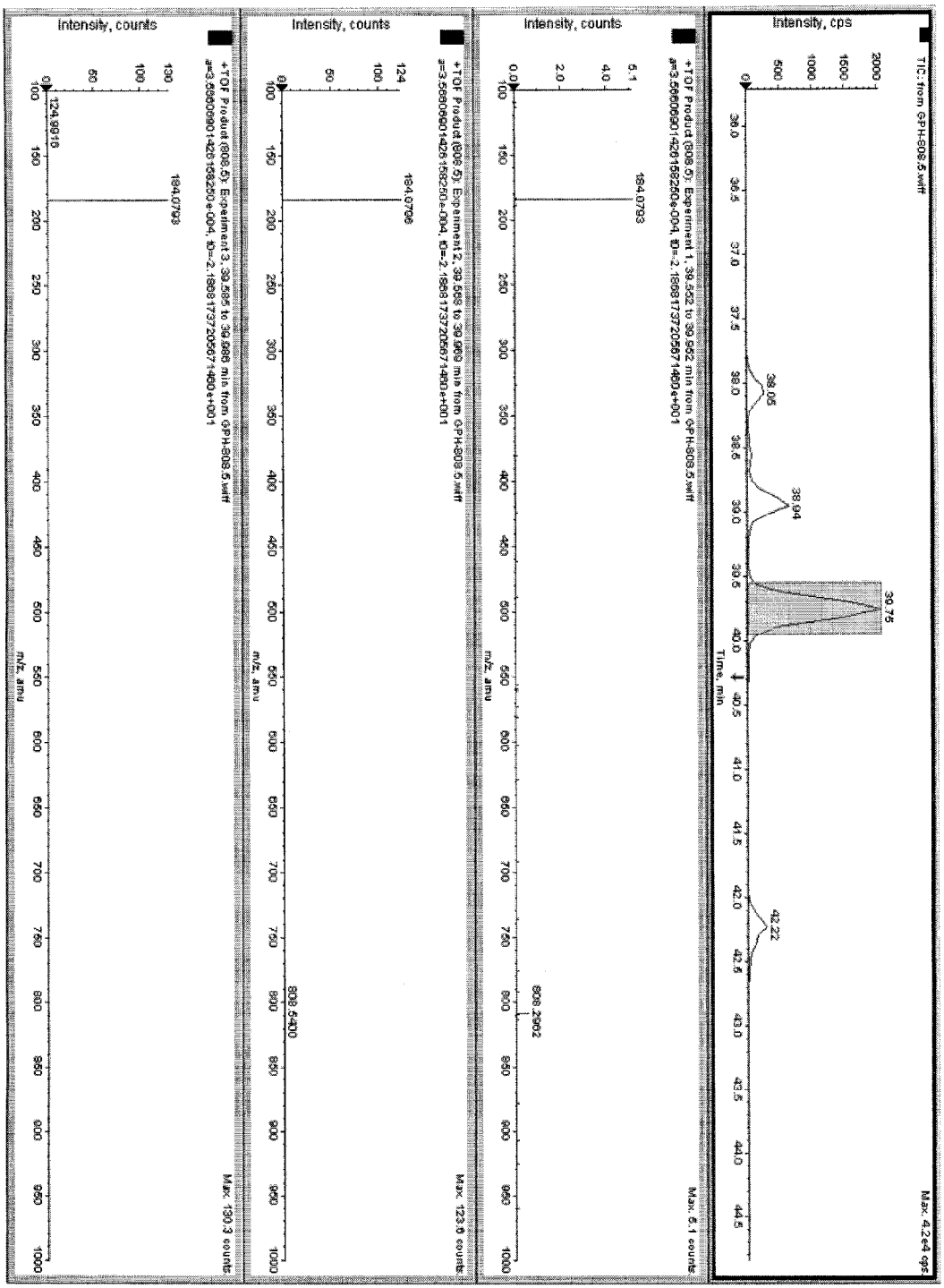


Figure 23 (Cont.)

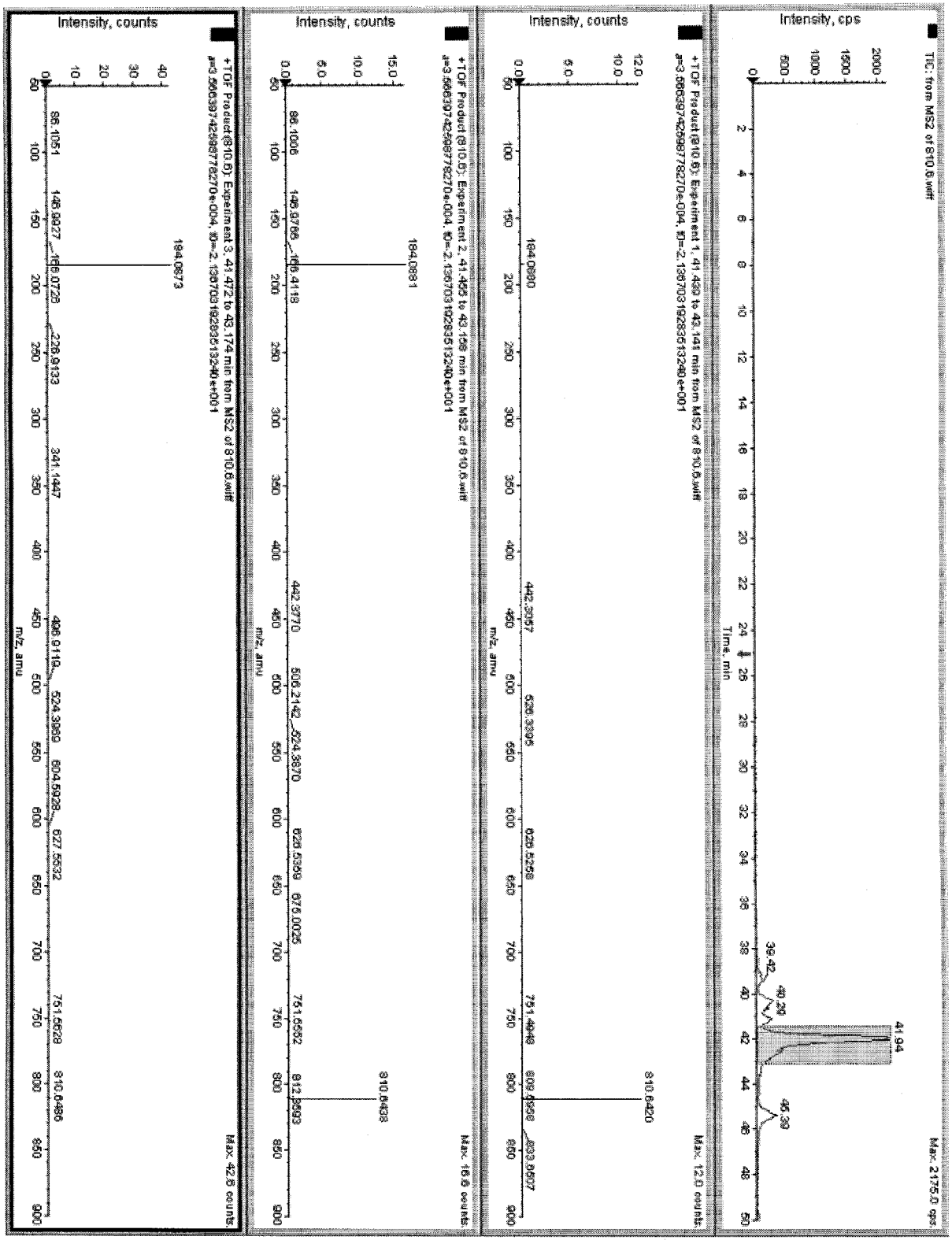

TIC: from MS2 of 810.6.wiff
Intensity, cps
Time, min
Max. 2175.0 cps.
39.42
40.29
41.94
45.39
+TOF Product (810.6): Experiment 1, 41.430 to 43.141 min from MS2 of 810.6.wiff
Intensity, counts
m/z, amu
Max. 12.0 counts.
184.0890
442.3057
526.3395
626.5258
751.4048
809.9958
893.8607
810.6420
+TOF Product (810.6): Experiment 2, 41.455 to 43.158 min from MS2 of 810.6.wiff
Max. 16.6 counts.
184.0881
98.1006
146.9765
166.4119
442.3770
506.2142
524.3870
626.5369
676.0025
751.6552
812.3693
810.6438
+TOF Product (810.6): Experiment 3, 41.472 to 43.174 min from MS2 of 810.6.wiff
Max. 42.5 counts.
184.0873
86.1051
146.9927
166.0726
226.9133
341.1447
406.9119
524.3969
604.5928
627.5532
751.6628
810.6486

Figure 24

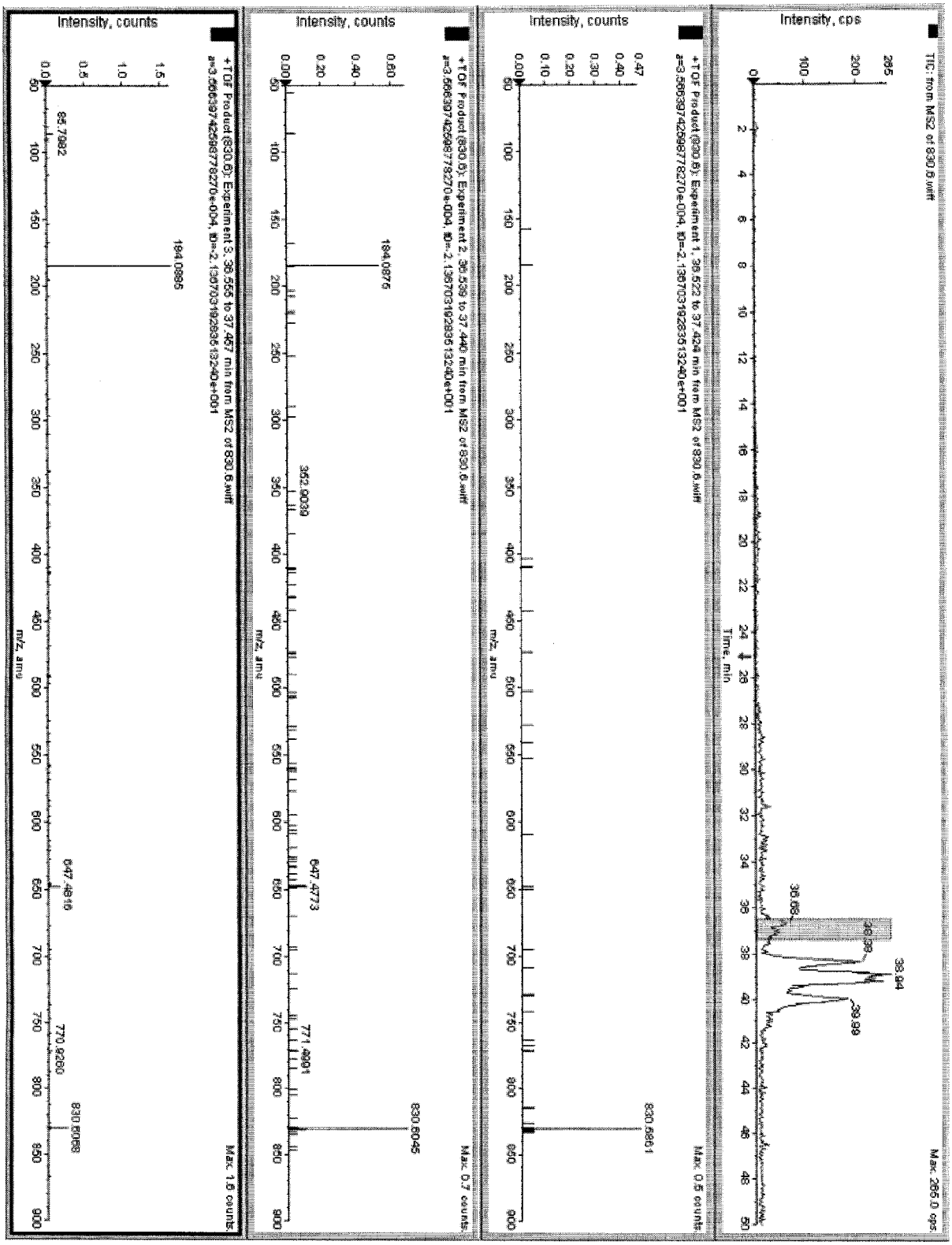

Intensity, cps
TIC: from MS2 of 830.6.wiff
Max: 265.0 cps.
36.68
36.98
38.94
39.99
Time, min
Intensity, counts
+TOF Product (830.6): Experiment 1, 35.622 to 37.424 min from MS2 of 830.6.wiff
Max: 0.5 counts.
830.5661
m/z, amu
Intensity, counts
+TOF Product (830.6): Experiment 2, 36.539 to 37.440 min from MS2 of 830.6.wiff
Max: 0.7 counts.
184.0876
352.9039
647.4773
771.4991
830.6045
m/z, amu
Intensity, counts
+TOF Product (830.6): Experiment 3, 36.565 to 37.467 min from MS2 of 830.6.wiff
Max: 1.5 counts.
84.7982
184.0886
647.4816
770.9260
830.6068
m/z, amu

Figure 25

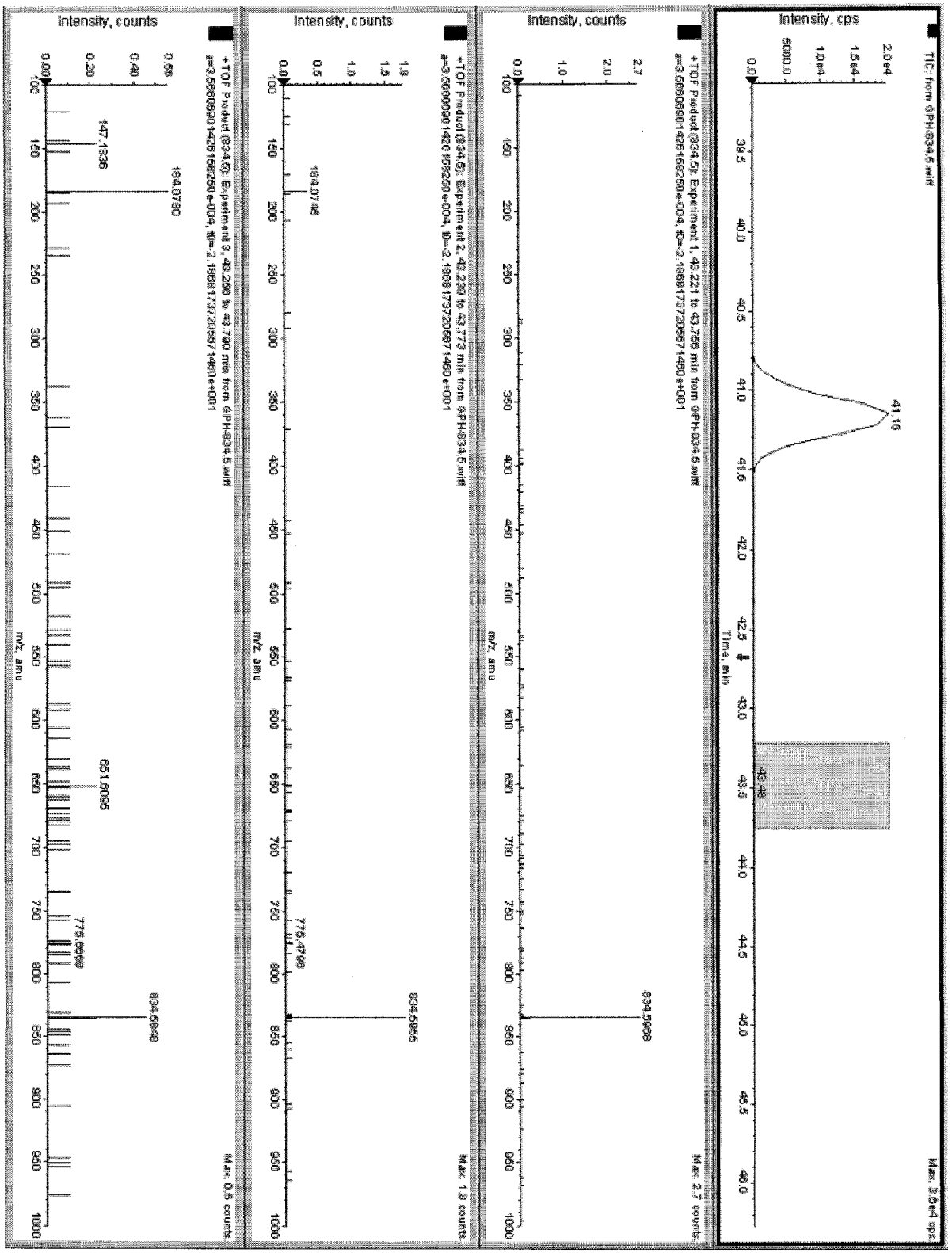

TIC: from 6PH-834.5.wiff
Intensity, cps
Time, min
41.16
43.38
Max. 3.6e4 cps.
+TOF Product (834.5): Experiment 1, 43.221 to 43.756 min from 6PH-834.5.wiff
Intensity, counts
m/z, amu
834.5998
Max. 2.7 counts.
+TOF Product (834.5): Experiment 2, 43.239 to 43.773 min from 6PH-834.5.wiff
Intensity, counts
m/z, amu
194.0745
775.4798
834.5955
Max. 1.8 counts.
+TOF Product (834.5): Experiment 3, 43.258 to 43.790 min from 6PH-834.5.wiff
Intensity, counts
m/z, amu
147.1836
194.0780
651.5065
775.5569
834.5948
Max. 0.5 counts.

Figure 26

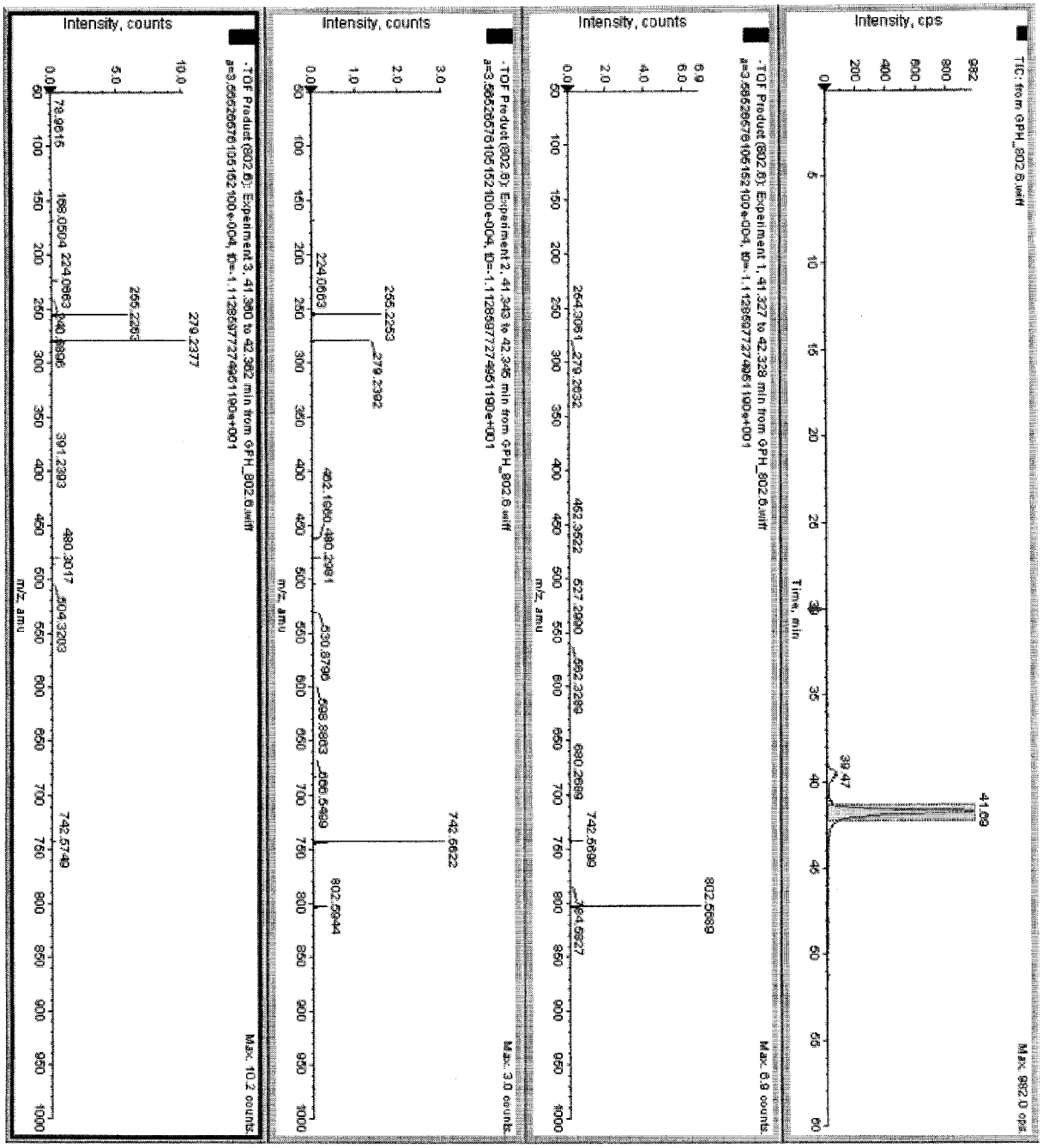

TIC: from GPH_802.6.wiff
Max. 982.0 cps
Intensity, cps
Time, min
41.09
39.47
Max. 5.8 counts
Intensity, counts
802.5689
742.5689
264.3081
279.2632
462.3622
527.2990
592.3289
680.2689
764.5827
Max. 3.0 counts
Intensity, counts
742.5622
224.0663
255.2253
279.2382
462.1680
480.2981
530.8796
598.8983
666.5499
802.5944
Max. 10.2 counts
Intensity, counts
279.2377
255.2283
224.0863
168.0504
78.9615
391.2393
480.3017
804.3203
742.5749
m/z, amu

Figure 27

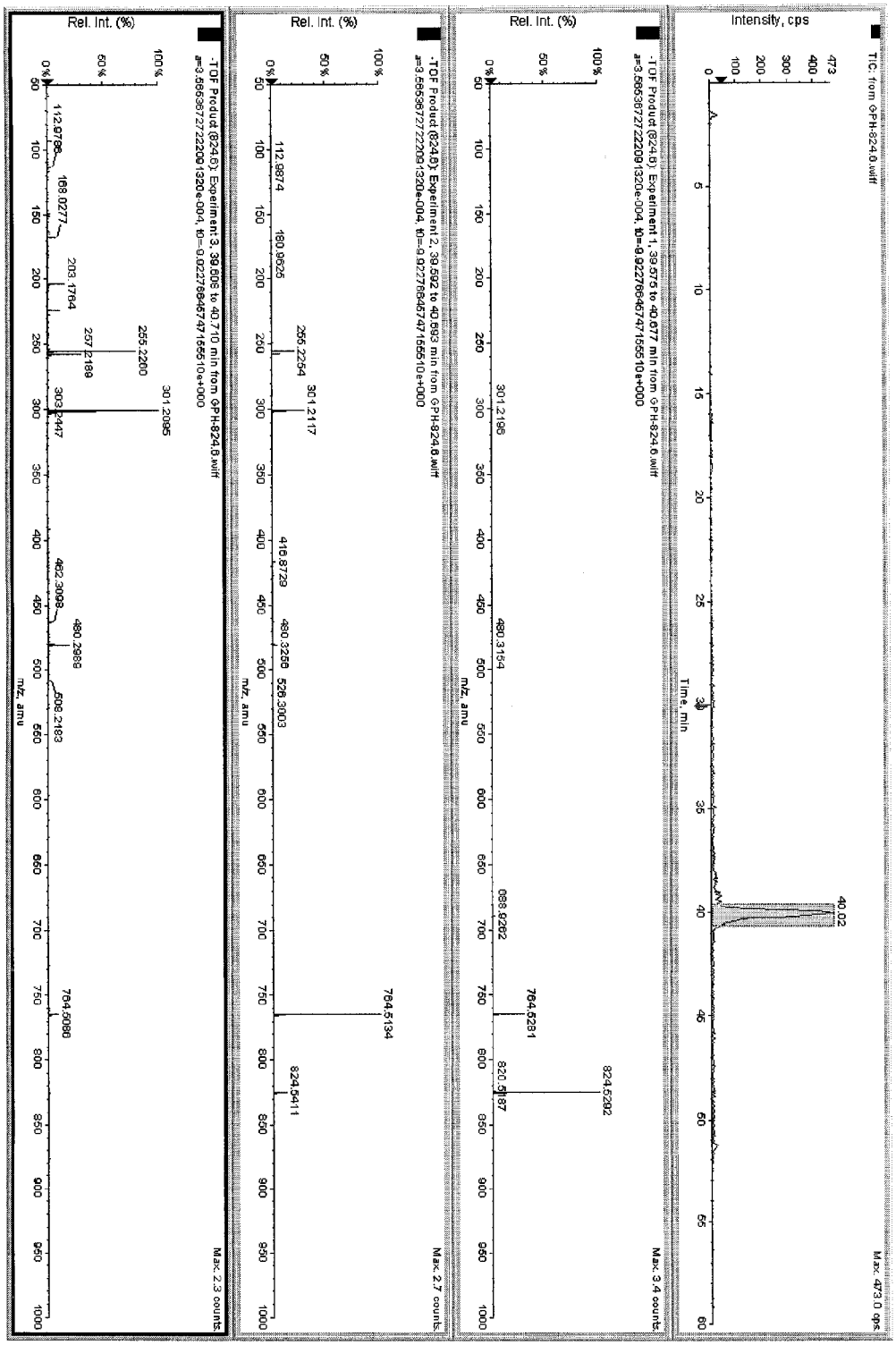

TIC: from GPH-824.6.wiff
Intensity, cps
Time, min
40.02
Max. 473.0 cps
-TOF Product (824.6): Experiment 1, 39.575 to 40.677 min from GPH-824.6.wiff
Rel. Int. (%)
m/z, amu
301.2196
480.3154
688.9282
764.5231
820.5187
824.5292
Max. 3.4 counts
-TOF Product (824.6): Experiment 2, 39.592 to 40.693 min from GPH-824.6.wiff
112.9874
180.9525
255.2254
301.2117
415.8729
480.3259
526.3003
764.5134
824.5411
Max. 2.7 counts
-TOF Product (824.6): Experiment 3, 39.606 to 40.710 min from GPH-824.6.wiff
112.9788
168.0277
203.1764
255.2260
257.2189
301.2085
303.2447
462.3098
480.2989
506.2183
764.5086
Max. 2.3 counts

Figure 28

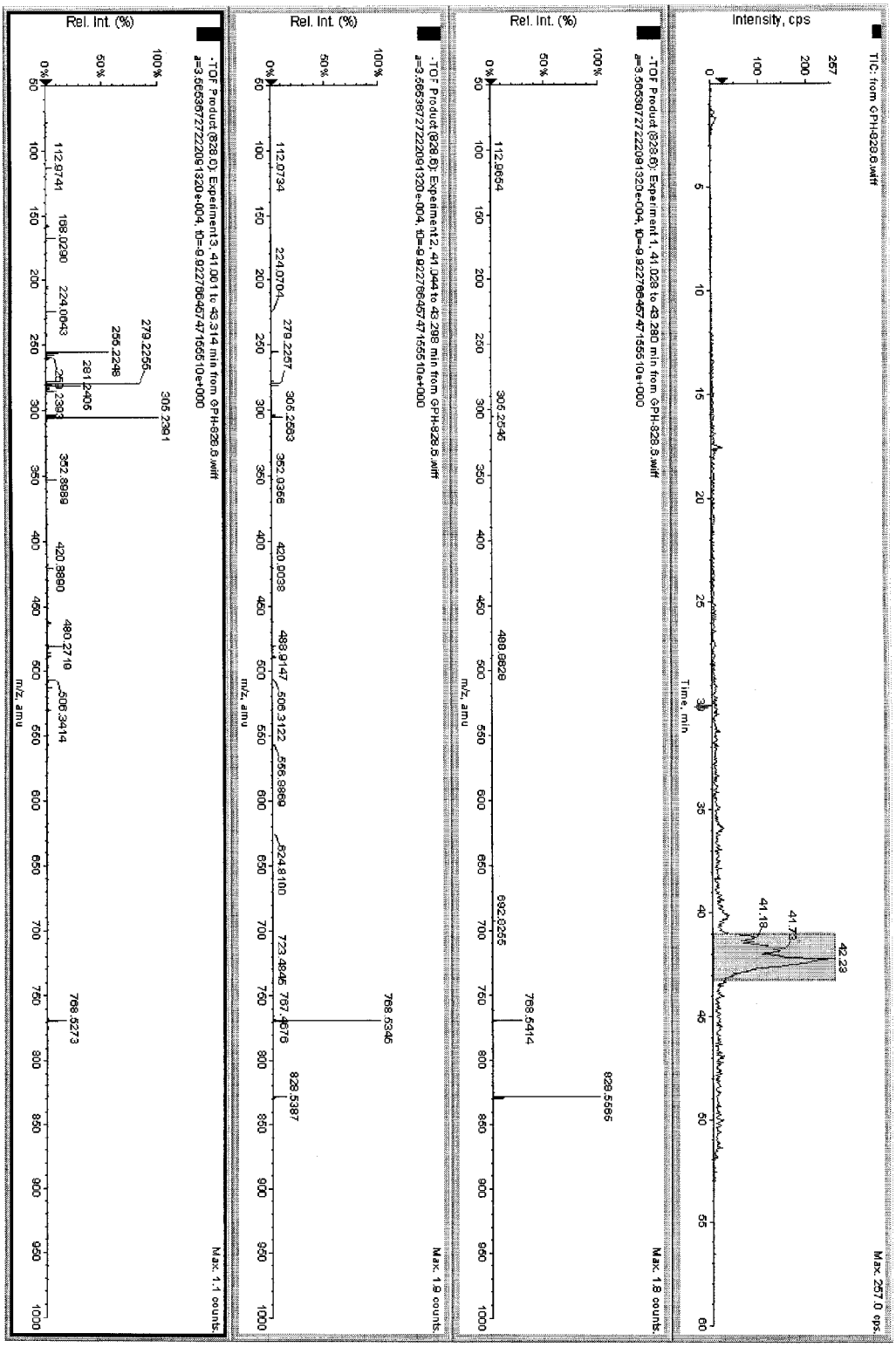

TIC: from GPH-828.6.wiff
Intensity, cps
Max. 257.0 cps.
Time, min
42.23
41.73
41.18
-TOF Product (828.6): Experiment 1, 41.028 to 43.280 min from GPH-828.5.wiff
Rel. Int. (%)
Max. 1.8 counts
112.9654
305.2546
488.9829
692.5255
768.5414
828.5565
-TOF Product (828.6): Experiment 2, 41.044 to 43.298 min from GPH-828.5.wiff
Rel. Int. (%)
Max. 1.9 counts
112.9734
224.0704
279.2257
305.2553
352.9366
420.9038
488.9147
506.3122
566.9869
724.4845
767.4676
768.5346
828.5387
-TOF Product (828.6): Experiment 3, 41.061 to 43.314 min from GPH-828.5.wiff
Rel. Int. (%)
Max. 1.1 counts
112.9741
168.0290
224.0643
255.2246
279.2255
305.2361
352.8989
420.8890
480.2719
506.3414
768.5273
m/z, amu

Figure 29

(a)

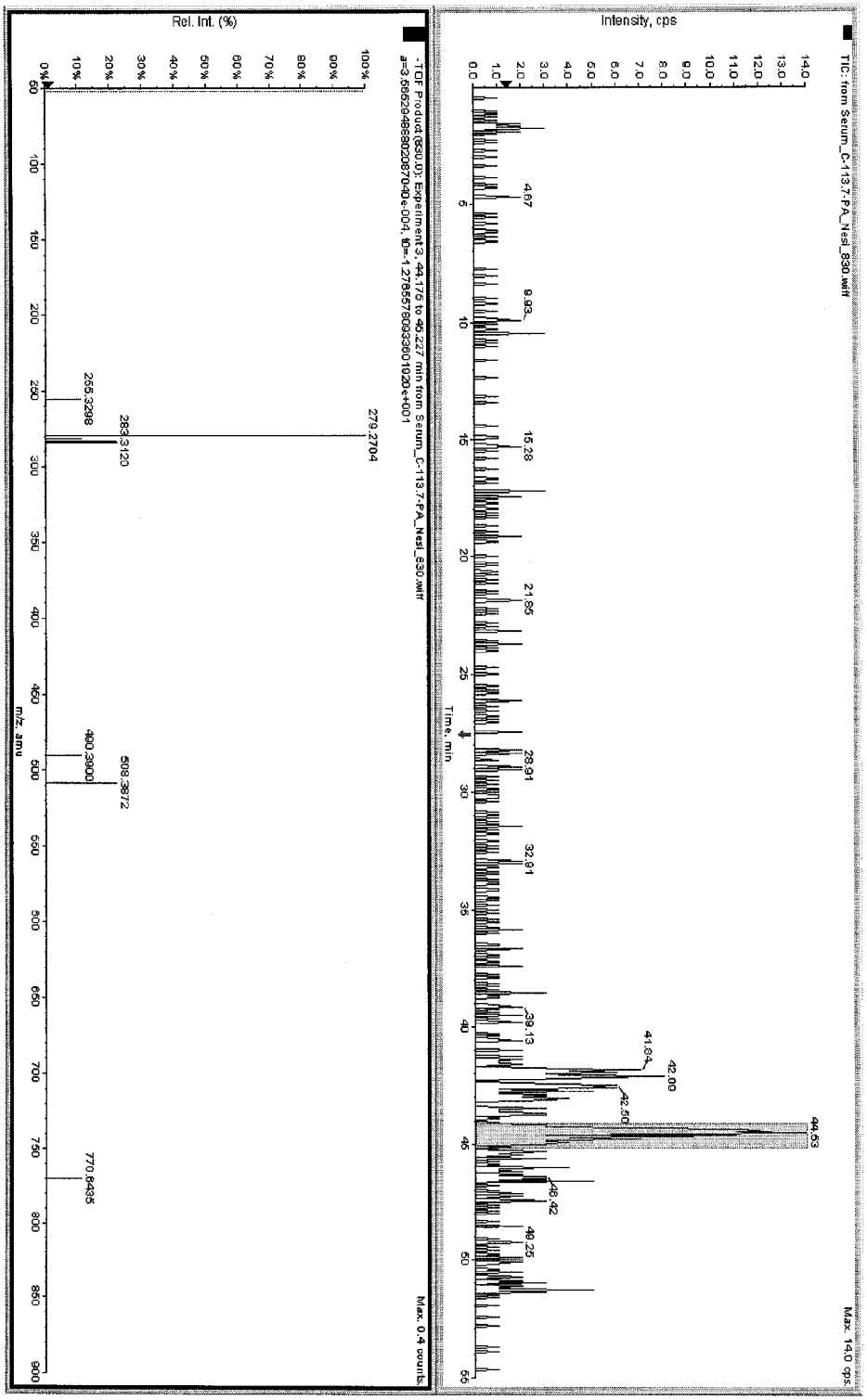

Intensity, cps
TIC: from Serum_C-113.7-PA_Nesl_830.wiff
Max. 14.0 cps
Time, min
4.67
9.93
15.28
21.85
28.91
32.91
39.13
41.64
42.09
42.50
44.53
46.42
49.25
Rel. Int. (%)
-TOF Product (830.0): Experiment 3, 44.176 to 45.227 min from Serum_C-113.7-PA_Nesl_830.wiff
a=3.56529488802067049e-004, to=-1.27855780933601920e+001
Max. 0.4 counts
m/z, amu
255.3298
283.3120
279.2704
490.3900
508.3872
770.5435

Figure 30

(b)

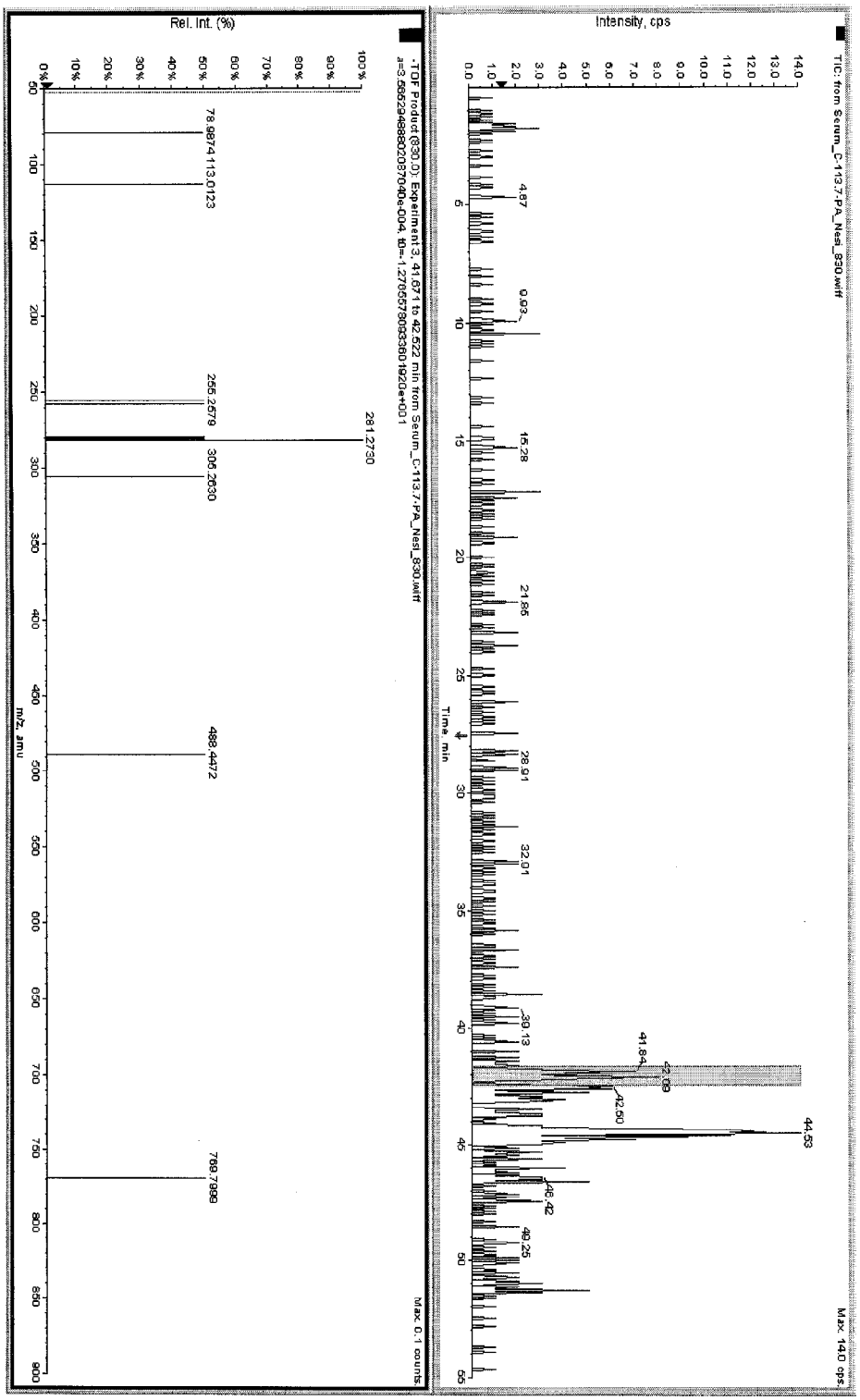


Figure 30 (cont.)

(a)

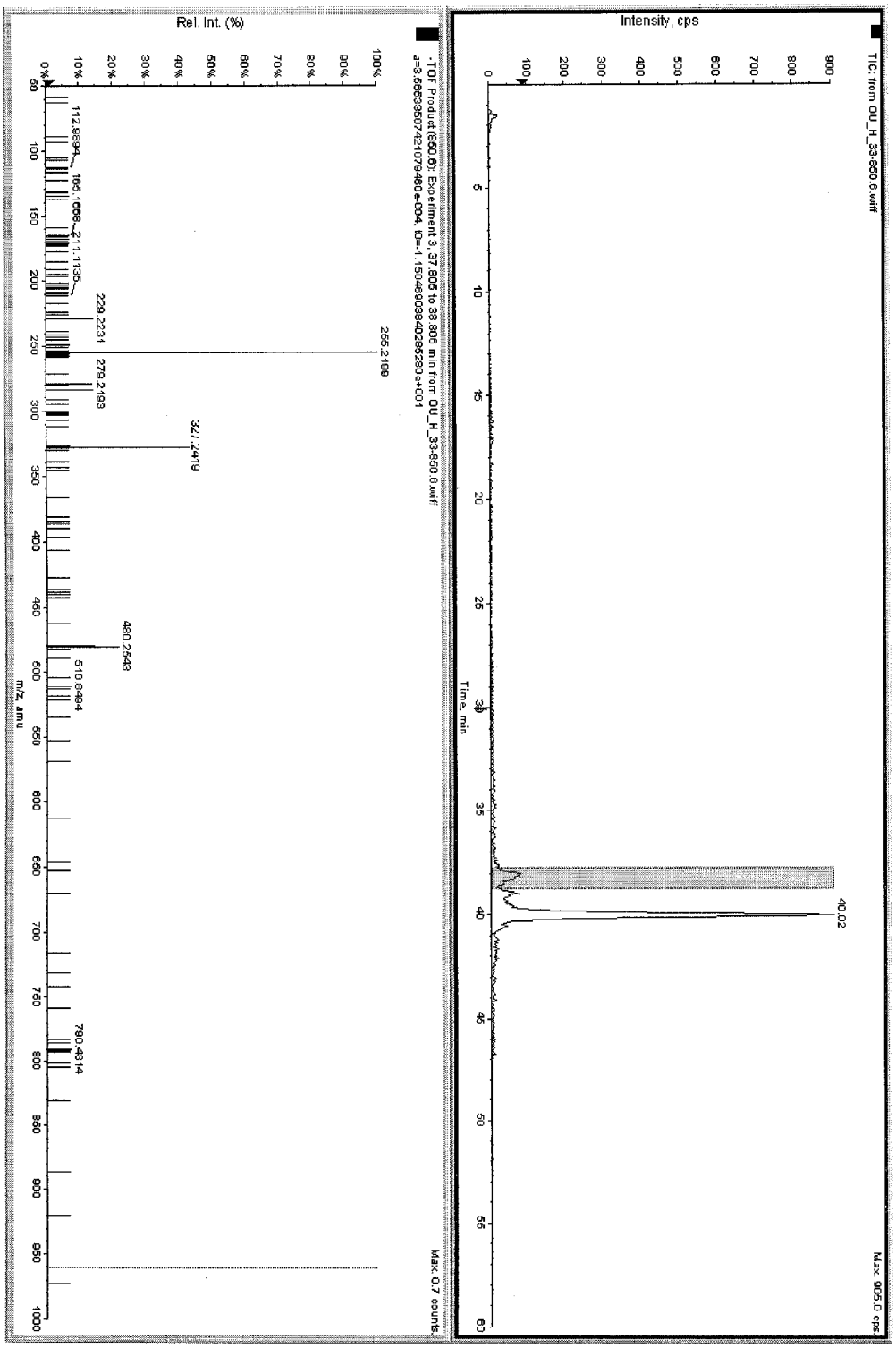

Rel. Int. (%)
m/z, amu
112.8894
165.1008
211.1135
229.2231
255.2109
279.2193
327.2419
480.2543
510.9464
790.4914
TIC: from DU_H_33-850.6.wiff
Intensity, cps
Time, min
40.02
Max. 906.0 cps
Max. 0.7 counts

Figure 31

(b)

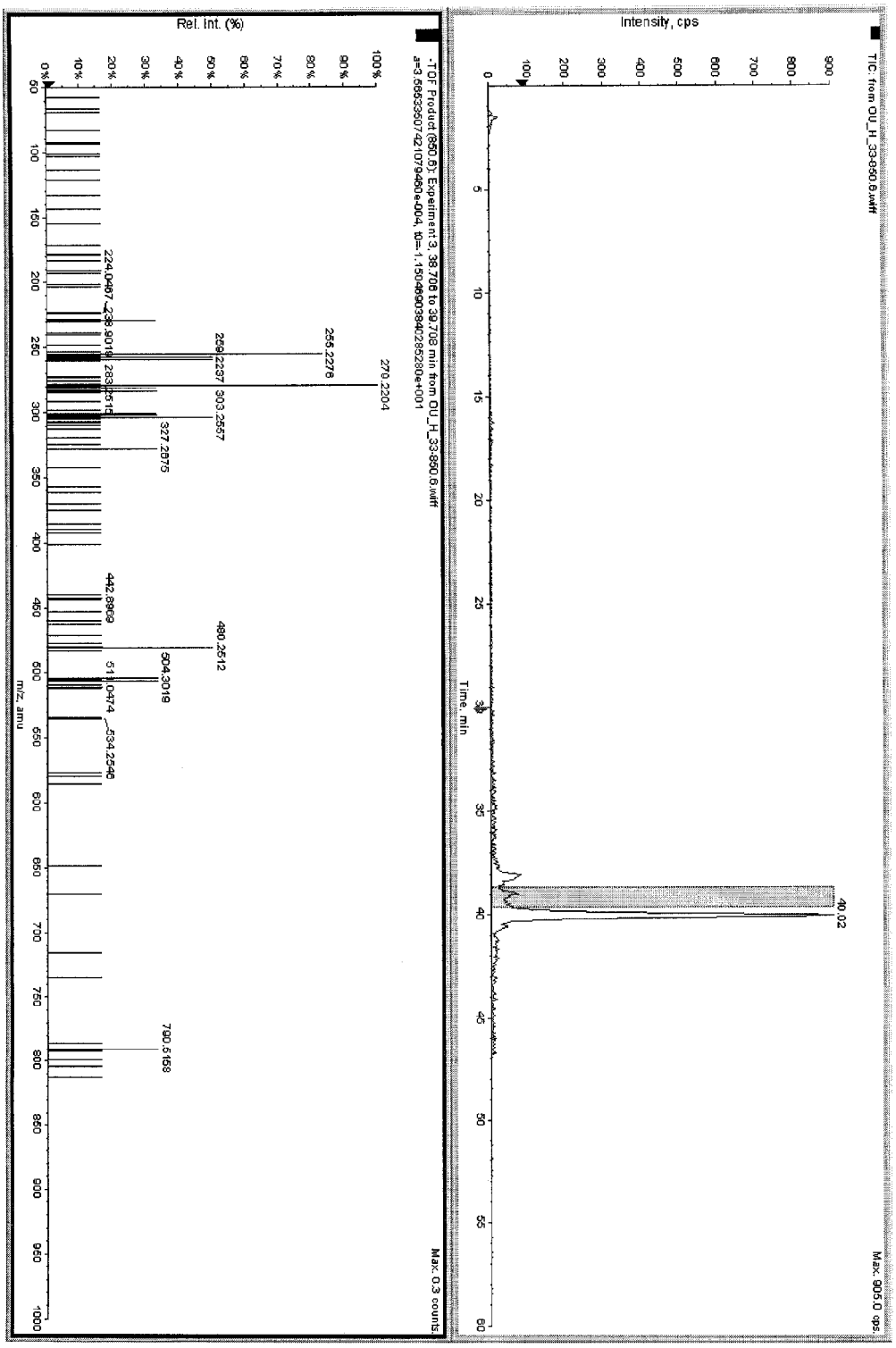


Figure 31 (cont.)

(c)

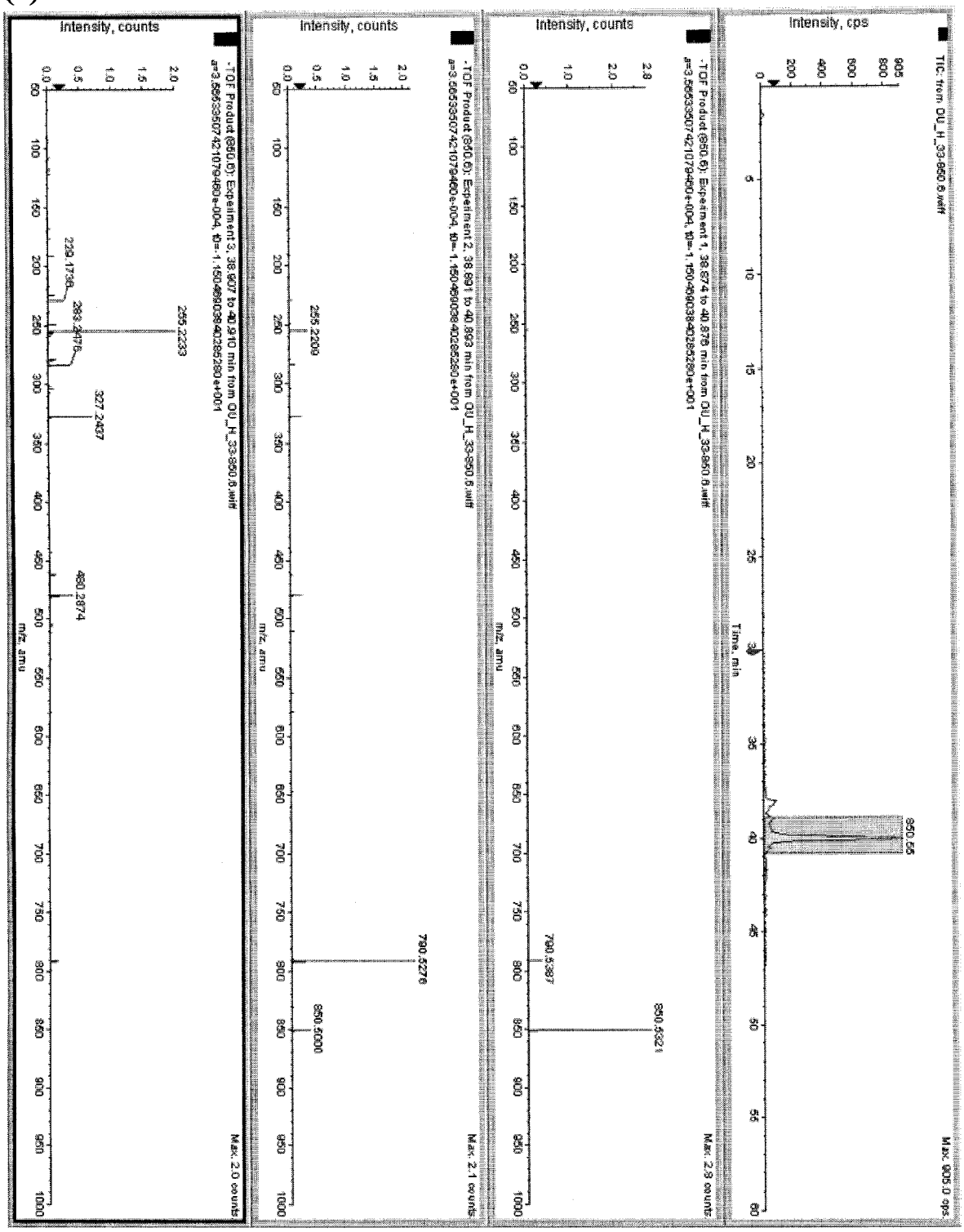


Figure 31 (cont.)

(d)

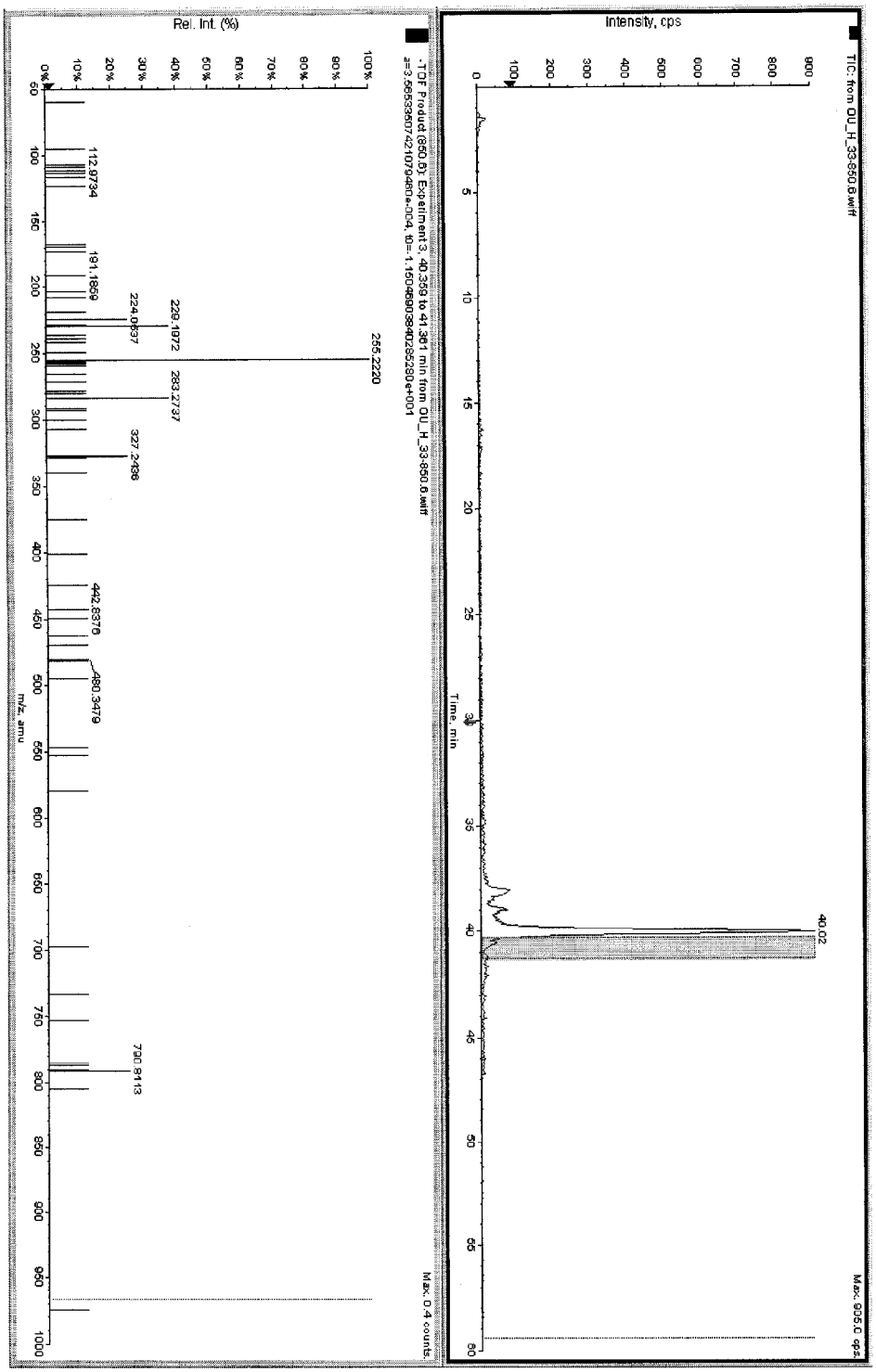


Figure 31 (cont.)

(a)

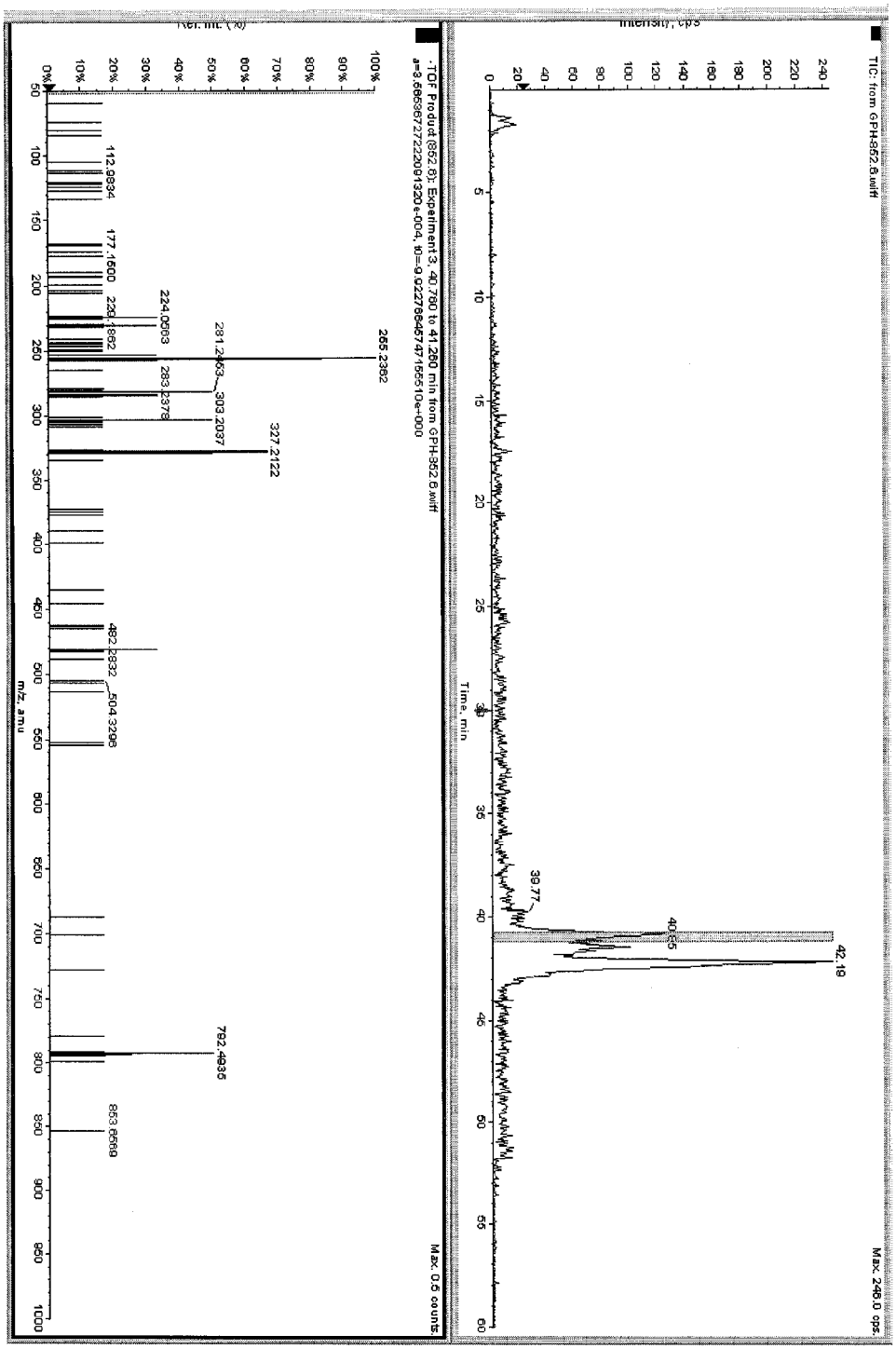

TIC: from GPH-862.6.wiff
Intensity, cps
Time, min
Max. 245.0 cps.
39.77
40.55
42.19
TOF Product (862.6): Experiment 3, 40.780 to 41.280 min from GPH-862.6.wiff
Max. 0.5 counts
m/z, amu
112.9834
177.1600
224.0563
255.2362
281.2453
283.2378
303.2037
327.2122
482.2932
504.3298
792.4935
853.5569

Figure 32

(b)

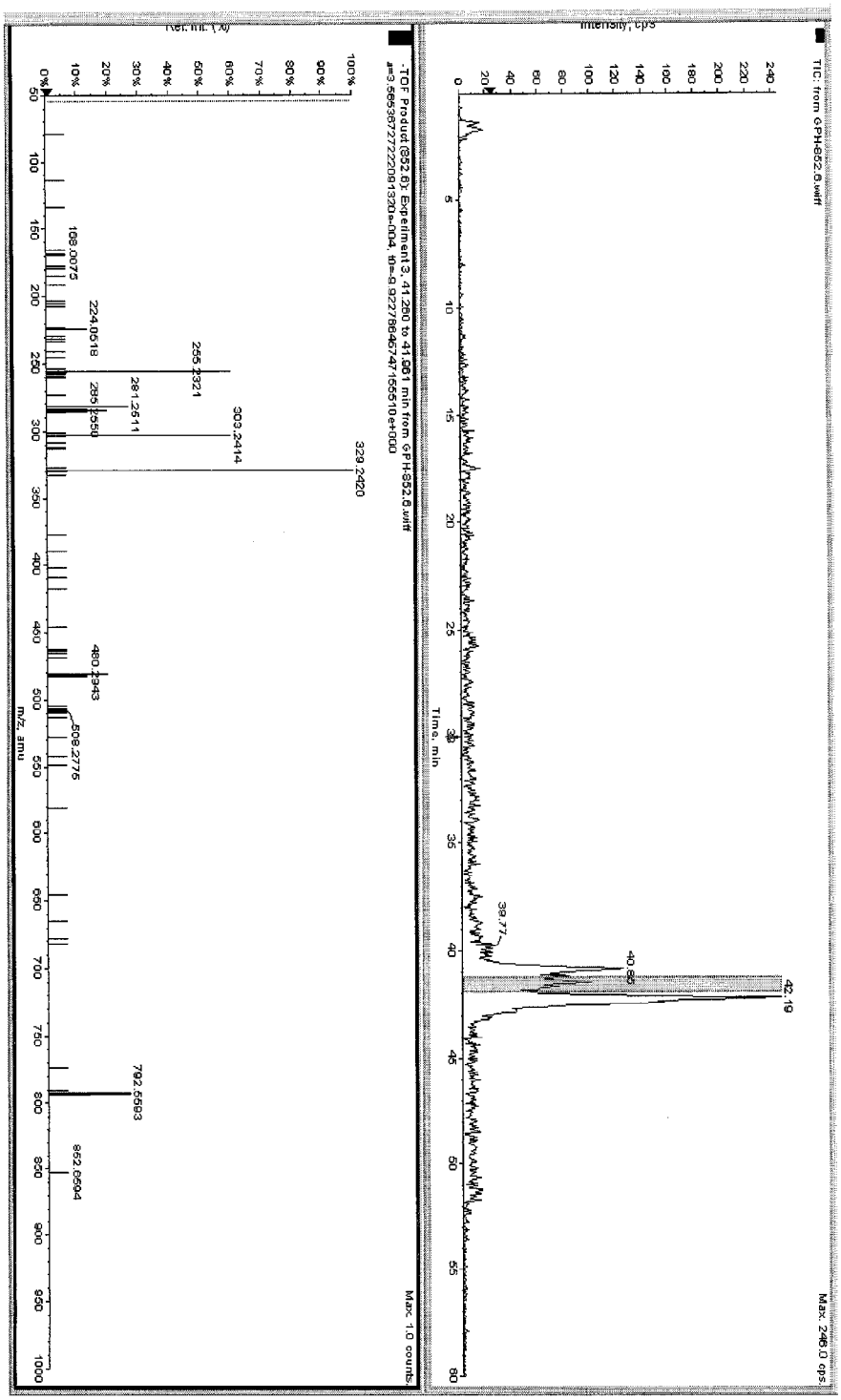


Figure 32 (cont.)

(c)

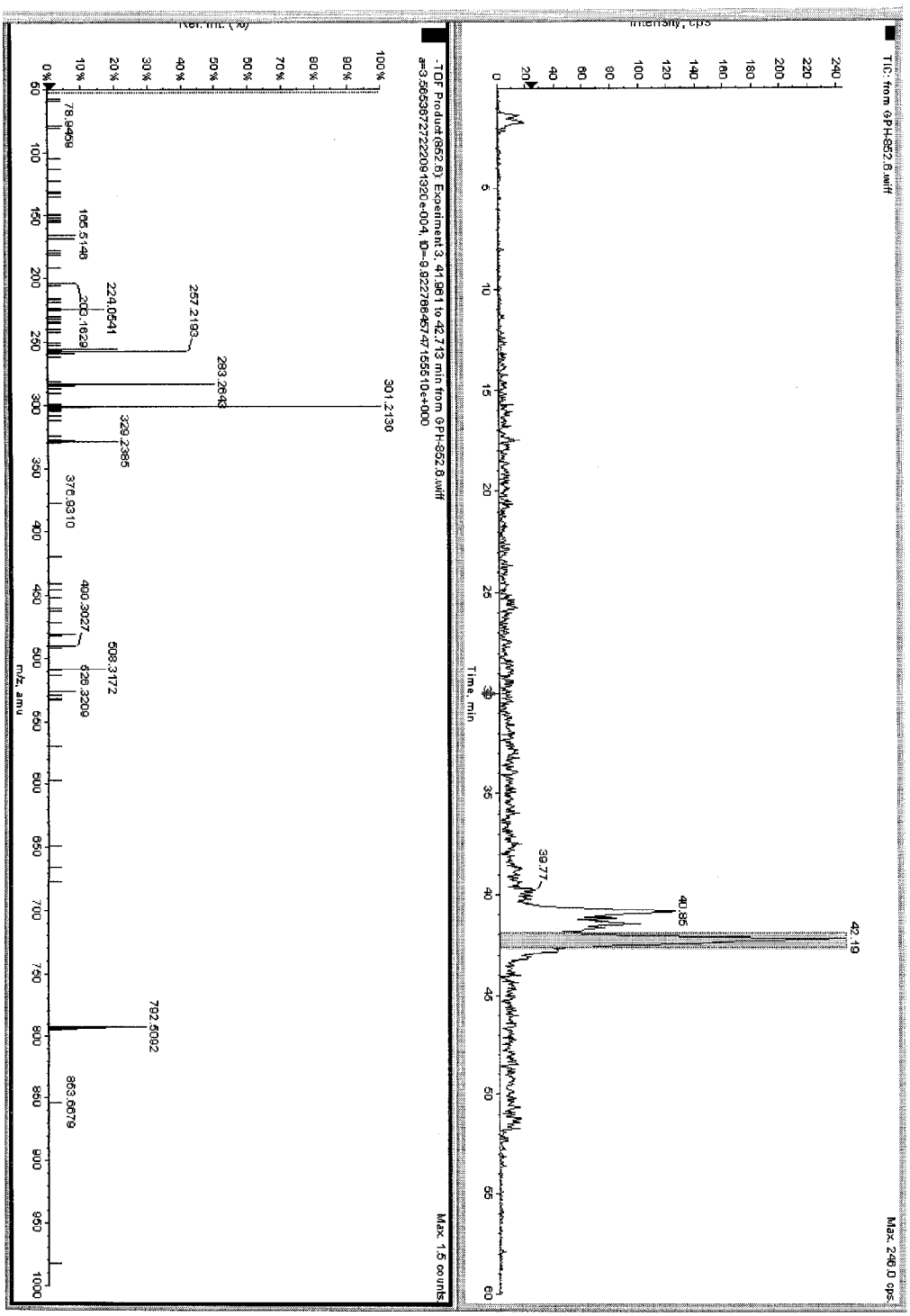


Figure 32 (cont.)

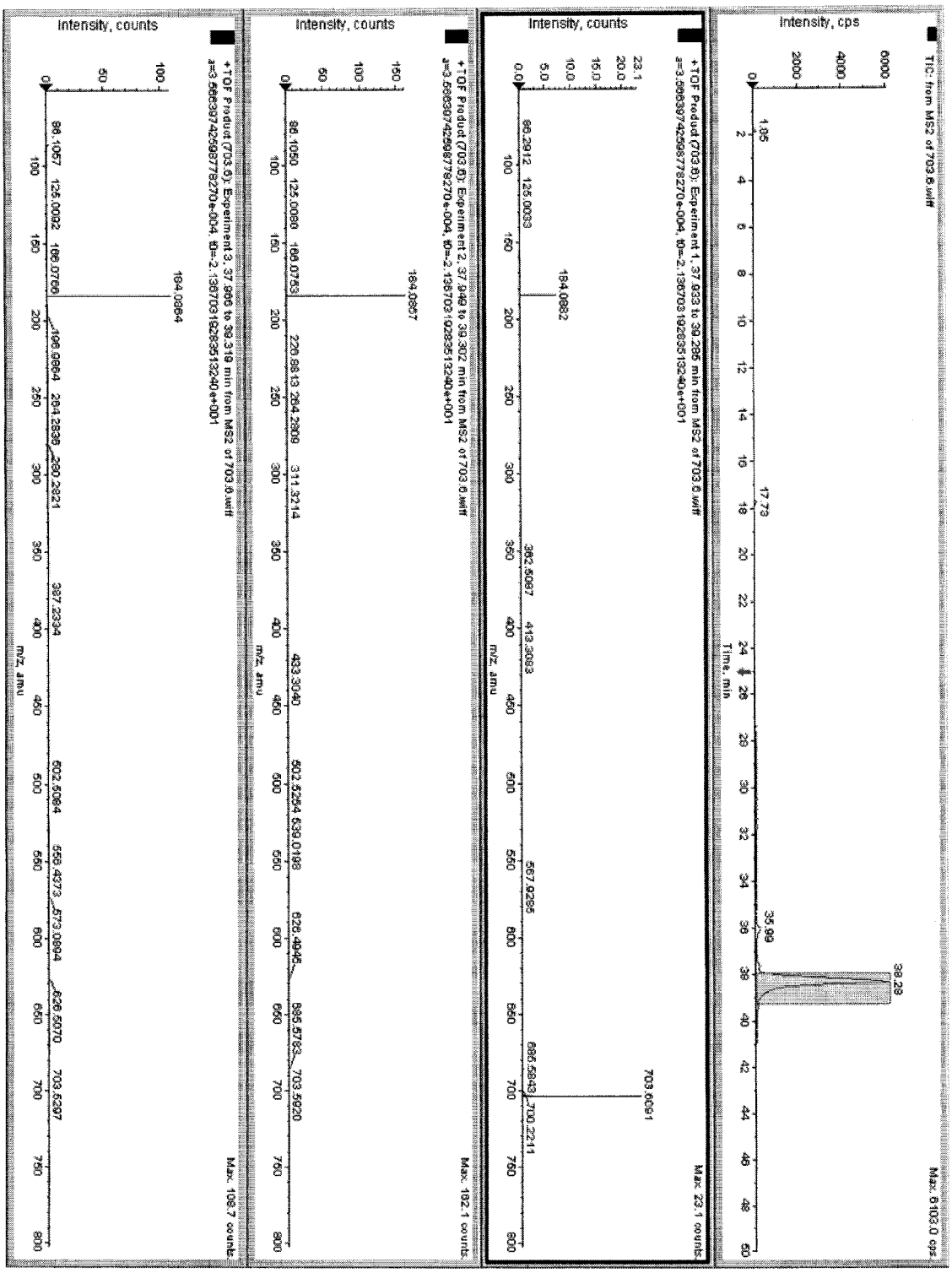

TIC: from MS2 of 703.6.wiff
Intensity, cps
Time, min
Max. 5103.0 cps
1.95
17.73
35.99
38.28
+TOF Product (703.6): Experiment 1, 37.933 to 39.295 min from MS2 of 703.6.wiff
Intensity, counts
m/z, amu
Max. 23.1 counts
96.2912
125.0033
184.0862
382.5087
413.3083
567.9295
685.5843
703.6091
+TOF Product (703.6): Experiment 2, 37.949 to 39.302 min from MS2 of 703.6.wiff
Max. 192.1 counts
96.1050
125.0089
168.0753
184.0857
226.9813
264.2809
311.3214
433.3040
602.5254
639.0198
626.4945
685.5783
703.5920
+TOF Product (703.6): Experiment 3, 37.966 to 39.319 min from MS2 of 703.6.wiff
Max. 108.7 counts
96.1057
125.0092
166.0756
184.0864
196.9864
264.2838
280.2821
387.2334
602.5084
559.4373
573.0994
626.5070
703.5397

Figure 33

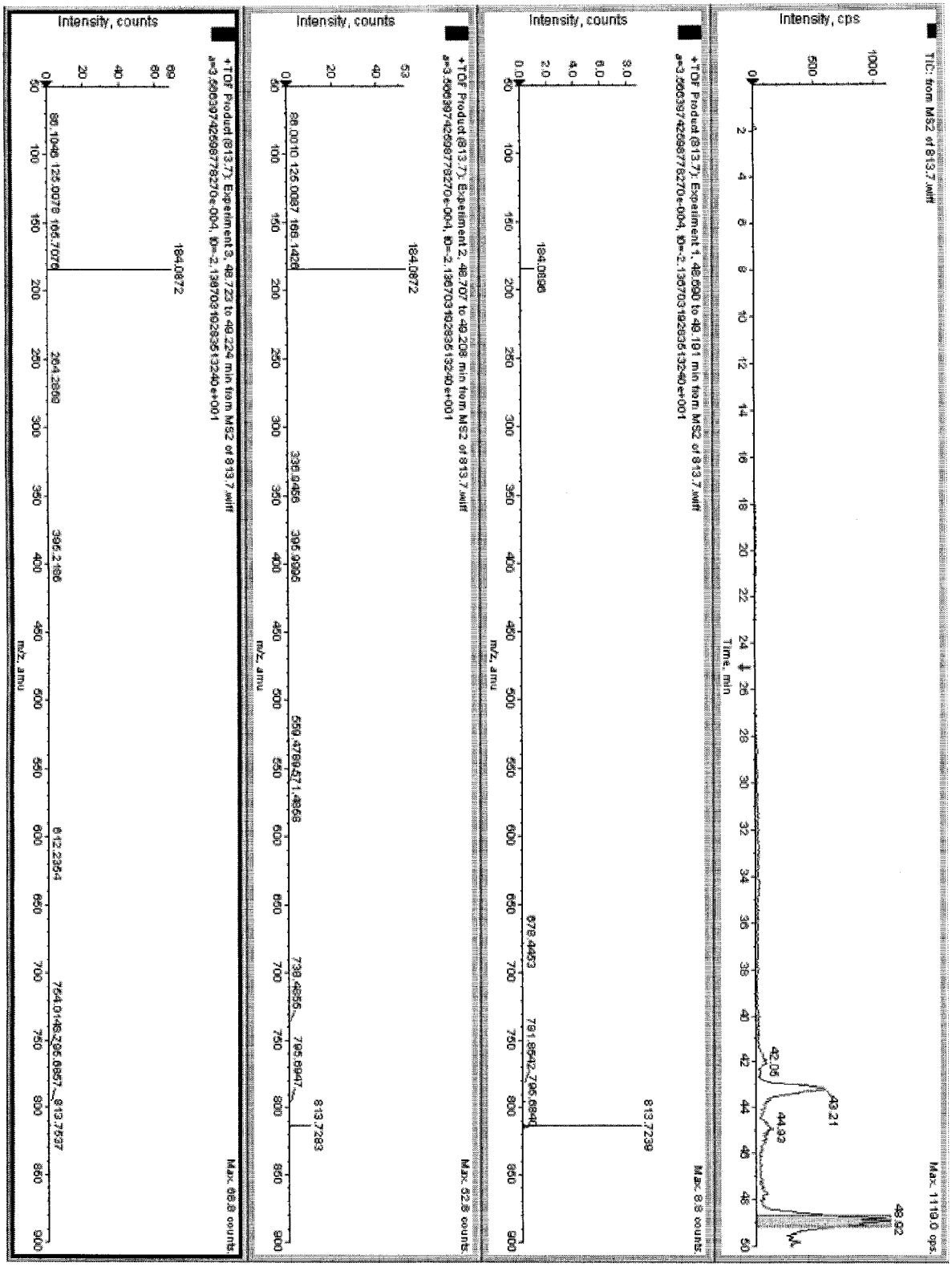

TIC: from MS2 of 813.7.wiff
Intensity, cps
Max. 1119.0 cps.
Time, min
+TOF Product (813.7): Experiment 1, 48.090 to 49.191 min from MS2 of 813.7.wiff
Intensity, counts
Max. 8.8 counts
m/z, amu
+TOF Product (813.7): Experiment 2, 48.707 to 49.208 min from MS2 of 813.7.wiff
Max. 52.8 counts
+TOF Product (813.7): Experiment 3, 48.723 to 49.224 min from MS2 of 813.7.wiff
Max. 66.8 counts

Figure 34

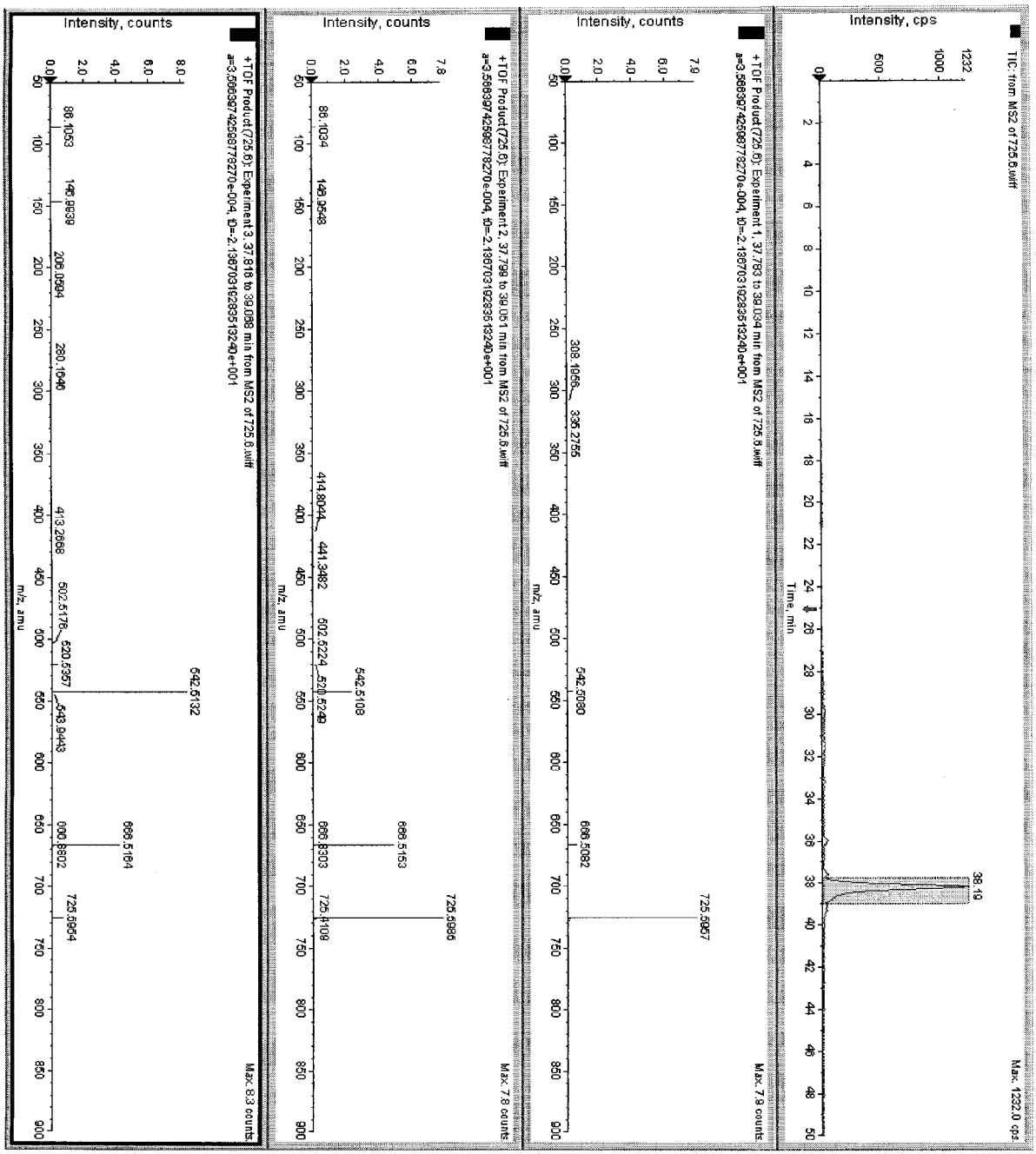

TIC: from MS2 of 725.8.wiff
Intensity, cps
Max. 1232.0 cps
38.19
Time, min
+TOF Product(725.8): Experiment 1, 37.783 to 39.034 min from MS2 of 725.8.wiff
Intensity, counts
Max. 7.9 counts
309.1956
335.2755
542.5080
666.5082
725.5957
+TOF Product(725.8): Experiment 2, 37.799 to 39.051 min from MS2 of 725.8.wiff
Intensity, counts
Max. 7.8 counts
88.1034
146.9548
414.8044
441.3482
502.5224
520.5249
542.5108
666.5163
725.5986
+TOF Product(725.8): Experiment 3, 37.816 to 39.068 min from MS2 of 725.8.wiff
Intensity, counts
Max. 8.3 counts
88.1053
146.9639
206.0894
280.1646
413.2668
502.5178
520.5357
542.5132
549.9443
666.5164
666.8802
725.5954
m/z, amu

Figure 35

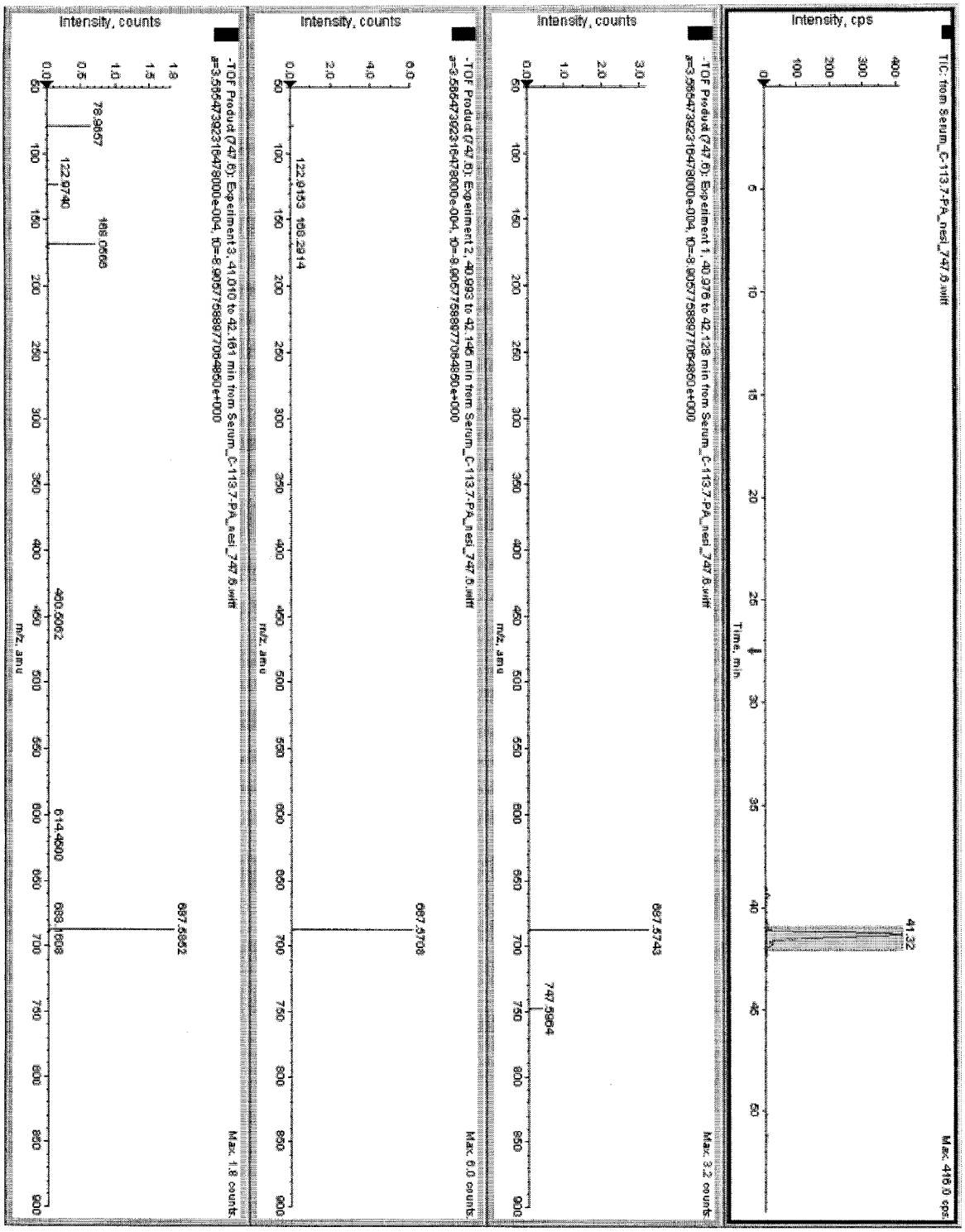

TIC: from Serum_C-113.7-PA_nesl_747.6.wiff
Intensity, cps
Time, min
Max: 416.0 cps.
41.32
-TOF Product (747.6): Experiment 1, 40.976 to 42.128 min from Serum_C-113.7-PA_nesl_747.6.wiff
Intensity, counts
m/z, amu
Max: 3.2 counts
887.5743
747.5964
-TOF Product (747.6): Experiment 2, 40.993 to 42.145 min from Serum_C-113.7-PA_nesl_747.6.wiff
Intensity, counts
m/z, amu
Max: 6.0 counts
887.5708
122.9153
168.2814
-TOF Product (747.6): Experiment 3, 41.010 to 42.161 min from Serum_C-113.7-PA_nesl_747.6.wiff
Intensity, counts
m/z, amu
Max: 1.8 counts
887.5662
614.4600
490.5062
168.0668
122.9740
78.9657

Figure 36

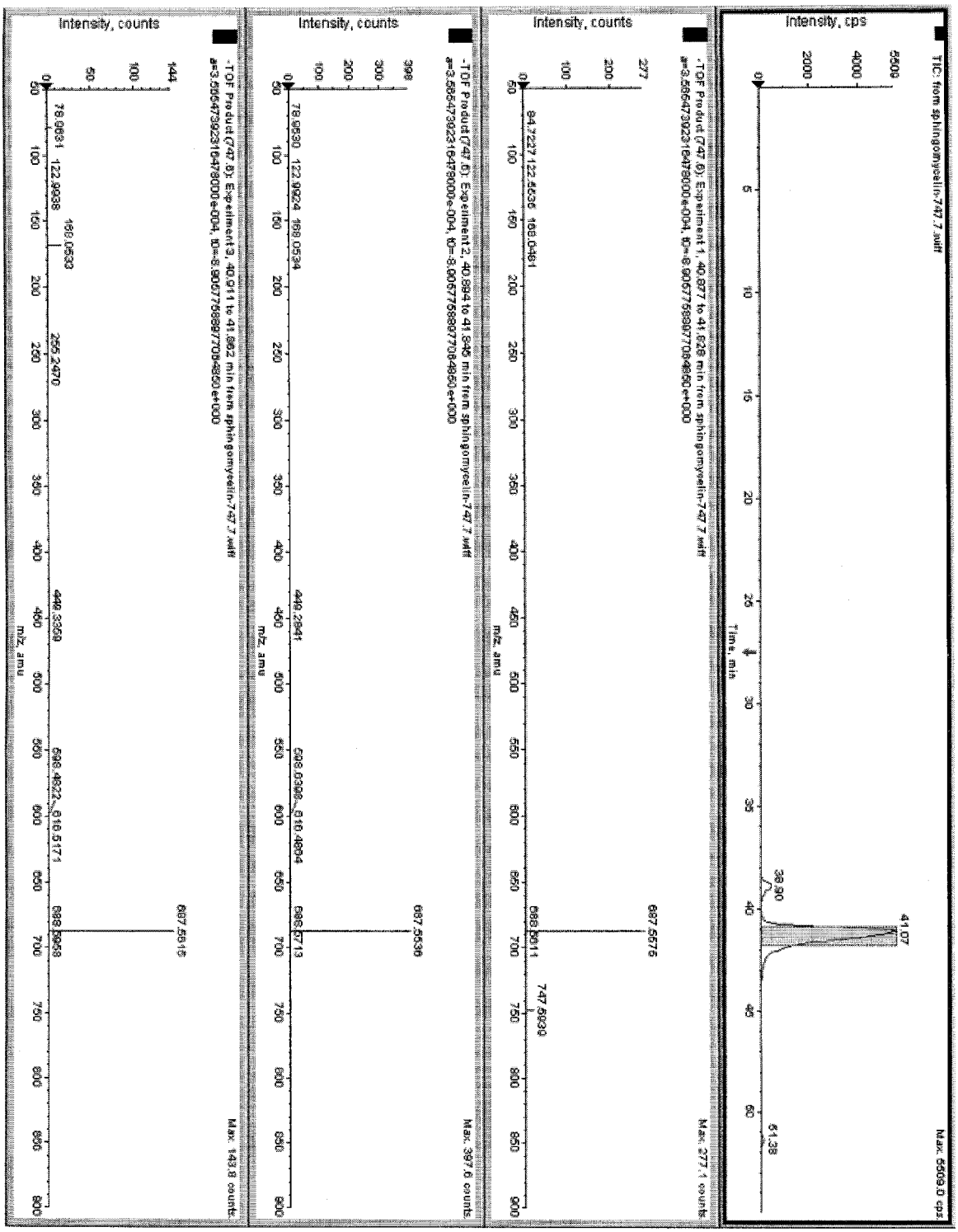

TIC: from sphingomyelin-747.7.wiff
Max. 5509.0 cps.
Intensity, cps
Time, min
41.07
38.90
51.38
-TOF Product (747.6): Experiment 1, 40.877 to 41.628 min from sphingomyelin-747.7.wiff
Max. 277.1 counts.
Intensity, counts
84.7227
122.4536
168.0461
667.5575
747.5939
-TOF Product (747.6): Experiment 2, 40.894 to 41.645 min from sphingomyelin-747.7.wiff
Max. 397.6 counts.
Intensity, counts
78.9830
122.9924
168.0534
449.2841
667.5536
-TOF Product (747.6): Experiment 3, 40.911 to 41.662 min from sphingomyelin-747.7.wiff
Max. 143.8 counts.
Intensity, counts
78.9831
122.9938
168.0533
255.2470
449.3359
667.5515
m/z, amu

Figure 37

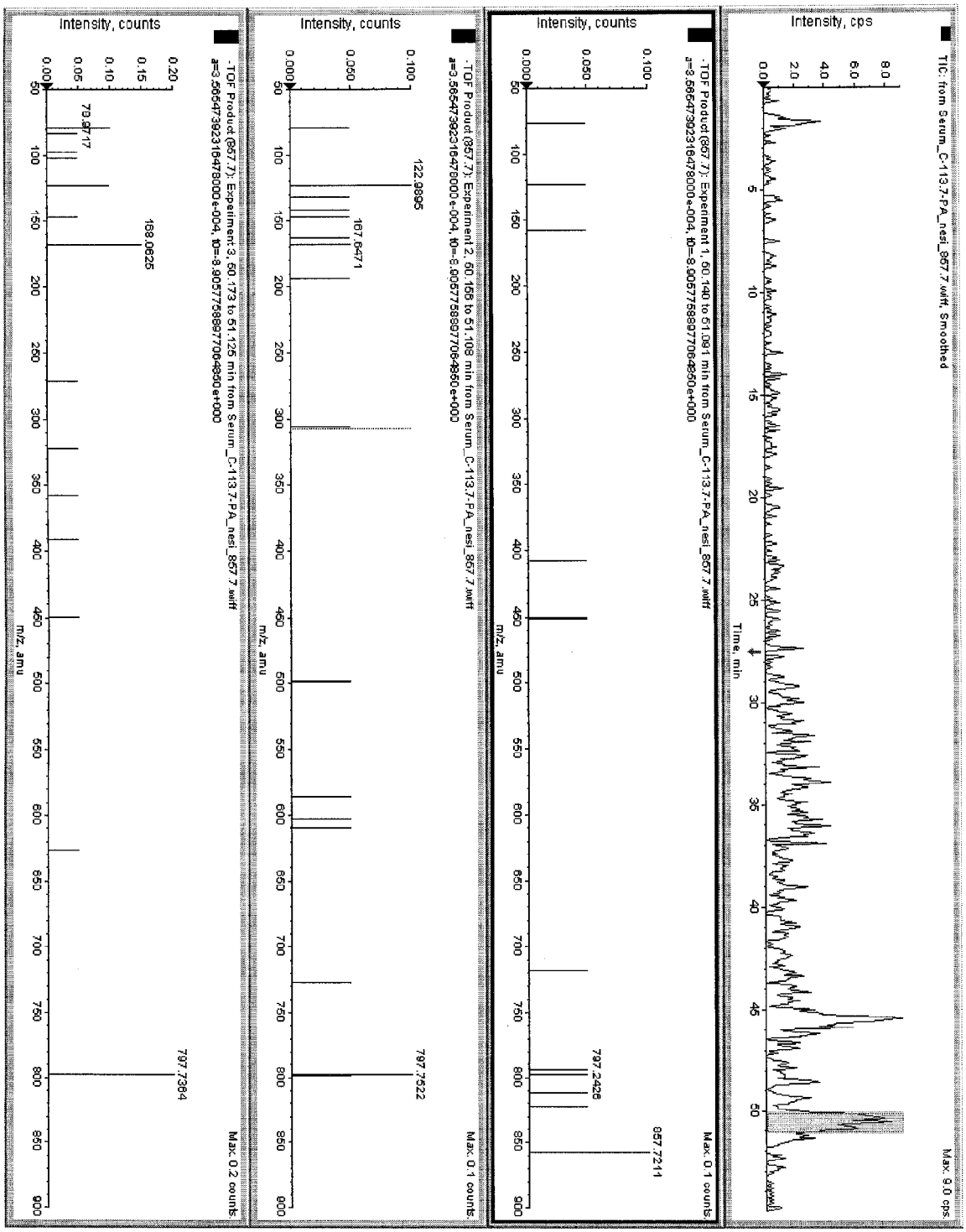

Intensity, cps
TIC: from Serum_C-113.7-PA_nesl_857.7.wiff, Smoothed
Max: 9.0 cps
Time, min
Intensity, counts
- TOF Product (857.7): Experiment 1, 60.140 to 51.091 min from Serum_C-113.7-PA_nesl_857.7.wiff
a=3.56547392316478000e-004, t0=-8.90577589977064850e+000
857.7211
797.2428
Max: 0.1 counts
m/z, amu
Intensity, counts
- TOF Product (857.7): Experiment 2, 60.158 to 51.108 min from Serum_C-113.7-PA_nesl_857.7.wiff
a=3.56547392316478000e-004, t0=-8.90577589977064850e+000
122.9895
167.8471
797.7522
Max: 0.1 counts
m/z, amu
Intensity, counts
- TOF Product (857.7): Experiment 3, 60.173 to 51.125 min from Serum_C-113.7-PA_nesl_857.7.wiff
a=3.56547392316478000e-004, t0=-8.90577589977064850e+000
79.9717
168.0625
797.7384
Max: 0.2 counts
m/z, amu

Figure 38

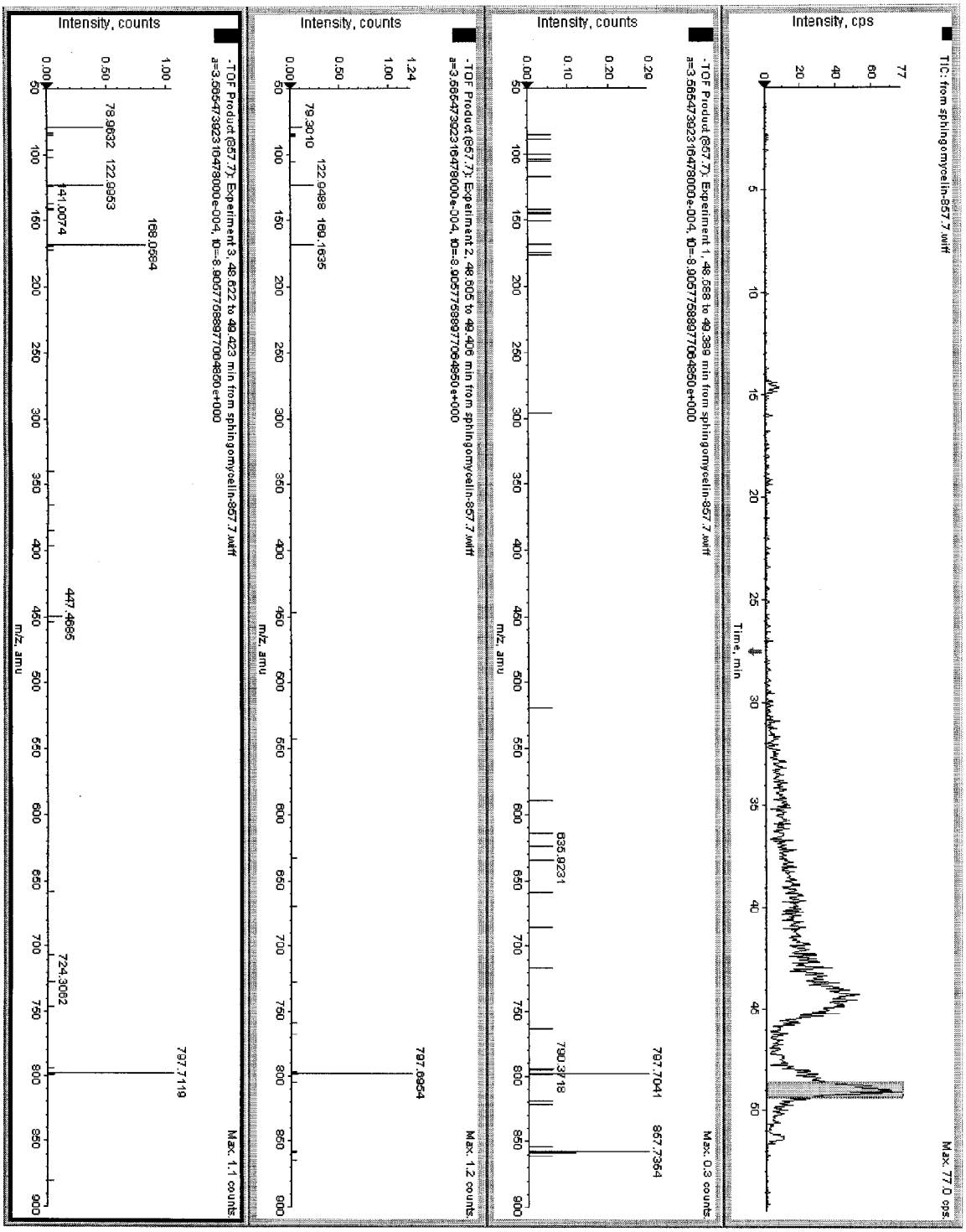

TIC: from sphingomyelin-857.7.wiff
Intensity, cps
Time, min
Max. 77.0 cps.
-TOF Product (857.7): Experiment 1, 48.568 to 49.389 min from sphingomyelin-857.7.wiff
Intensity, counts
m/z, amu
Max. 0.3 counts.
797.7041
857.7354
835.9231
790.3718
-TOF Product (857.7): Experiment 2, 48.605 to 49.406 min from sphingomyelin-857.7.wiff
Intensity, counts
m/z, amu
Max. 1.2 counts.
797.6954
79.3010
122.9488
180.1635
-TOF Product (857.7): Experiment 3, 48.622 to 49.423 min from sphingomyelin-857.7.wiff
Intensity, counts
m/z, amu
Max. 1.1 counts.
797.7119
724.3062
447.4685
168.0594
79.9632
122.9963
141.0074

Figure 39

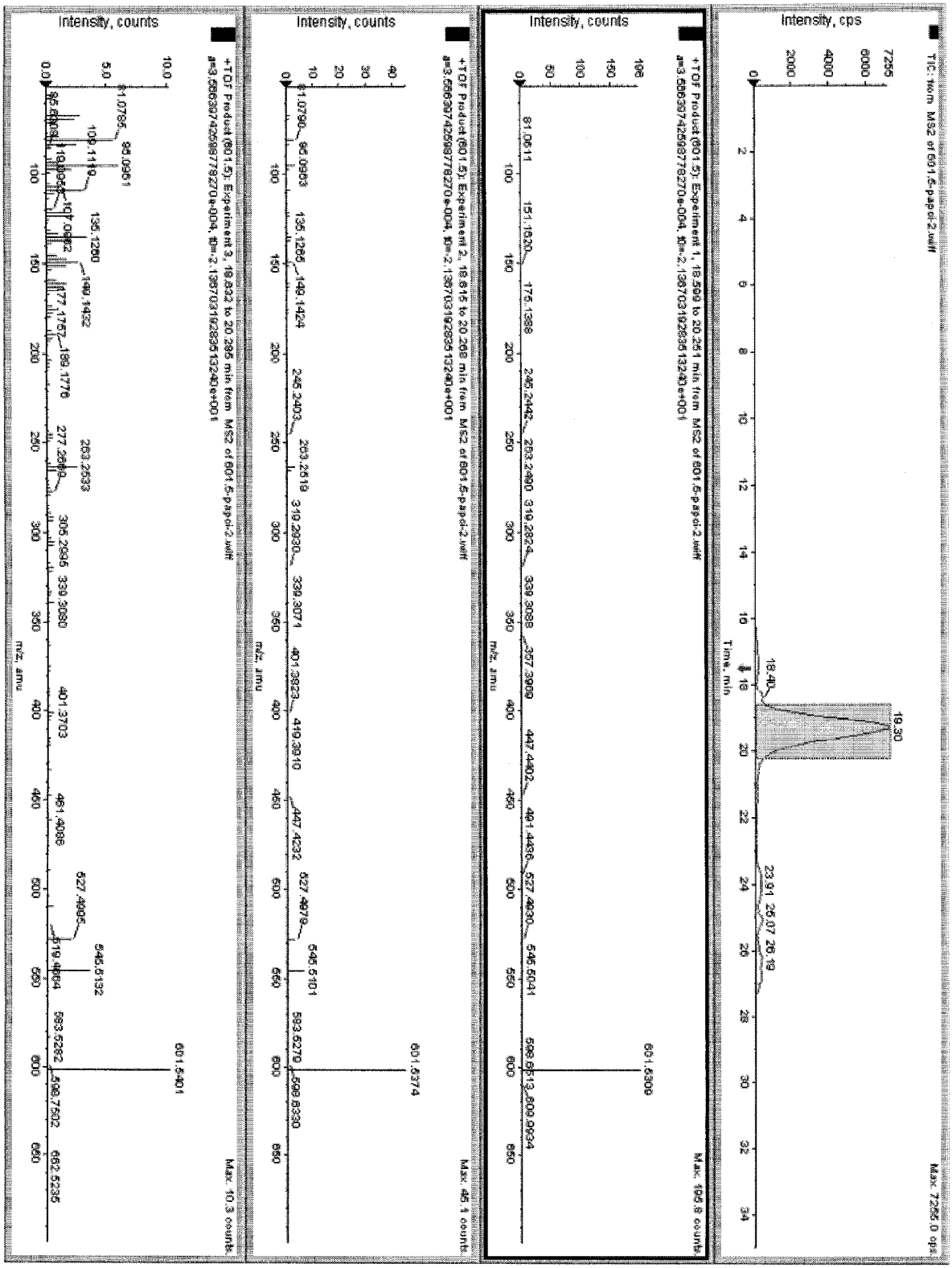
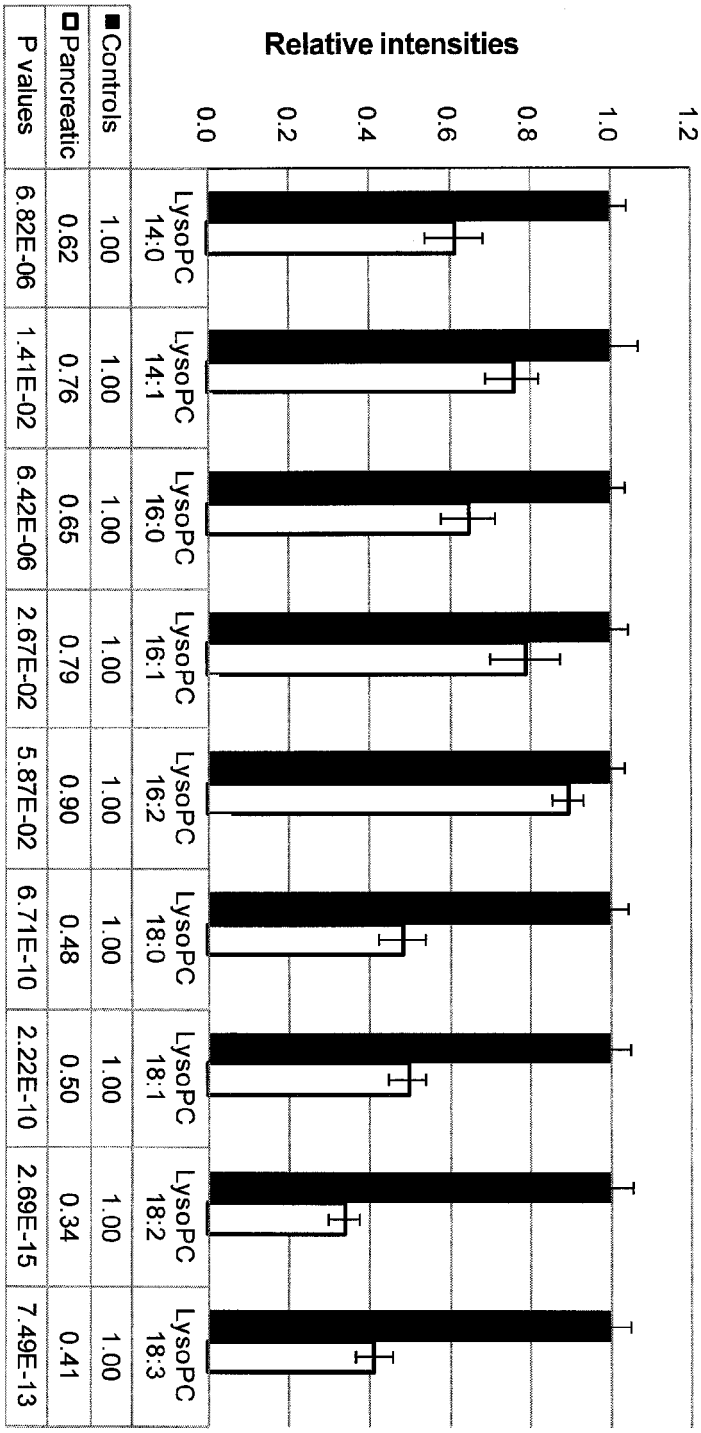

Intensity, cps
Time, min
Intensity, counts
m/z, amu
18.40
19.30
23.91
25.07
26.19
601.6309
601.6374
601.6401

Figure 40

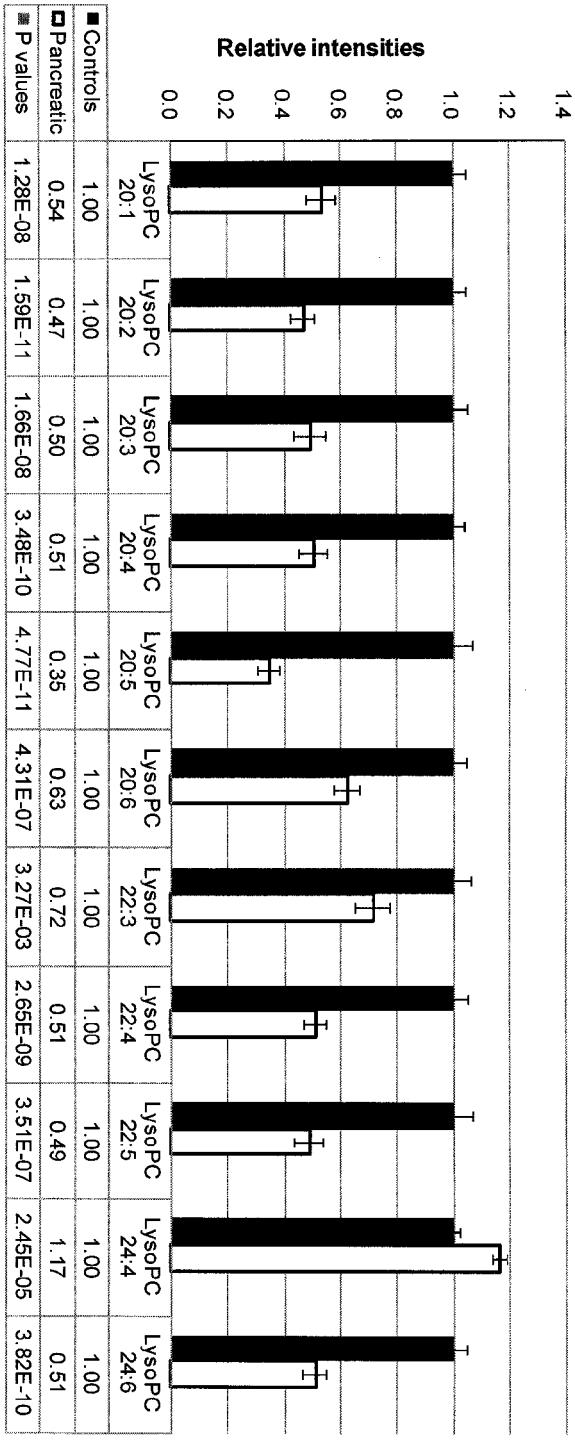
(a)



	LysoPC 14:0	LysoPC 14:1	LysoPC 16:0	LysoPC 16:1	LysoPC 16:2	LysoPC 18:0	LysoPC 18:1	LysoPC 18:2	LysoPC 18:3
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic	0.62	0.76	0.65	0.79	0.90	0.48	0.50	0.34	0.41
P values	6.82E-06	1.41E-02	6.42E-06	2.67E-02	5.87E-02	6.71E-10	2.22E-10	2.69E-15	7.49E-13

Figure 41

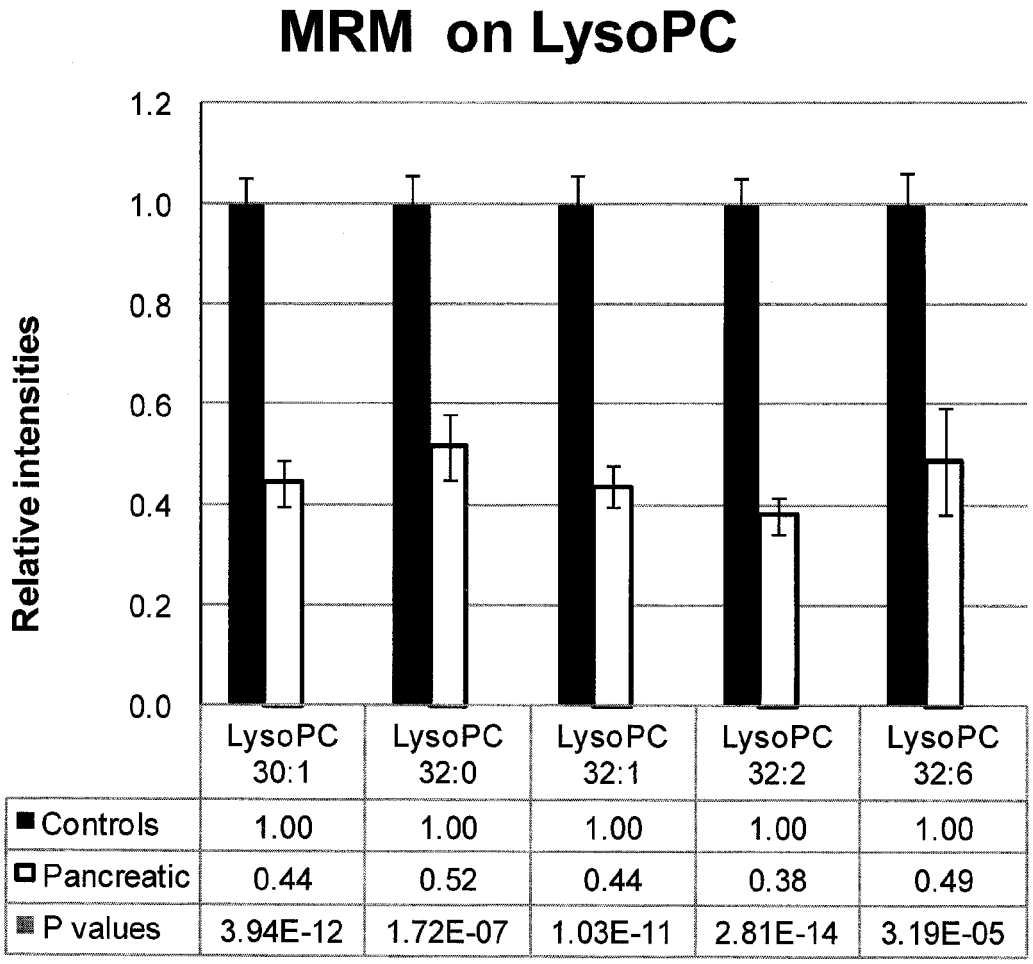
(b)



	LysoPC 20:1	LysoPC 20:2	LysoPC 20:3	LysoPC 20:4	LysoPC 20:5	LysoPC 20:6	LysoPC 22:3	LysoPC 22:4	LysoPC 22:5	LysoPC 24:4	LysoPC 24:6
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic	0.54	0.47	0.50	0.51	0.35	0.63	0.72	0.51	0.49	1.17	0.51
■ P values	1.28E-08	1.59E-11	1.66E-08	3.48E-10	4.77E-11	4.31E-07	3.27E-03	2.65E-09	3.51E-07	2.45E-05	3.82E-10

Figure 41 (Cont.)

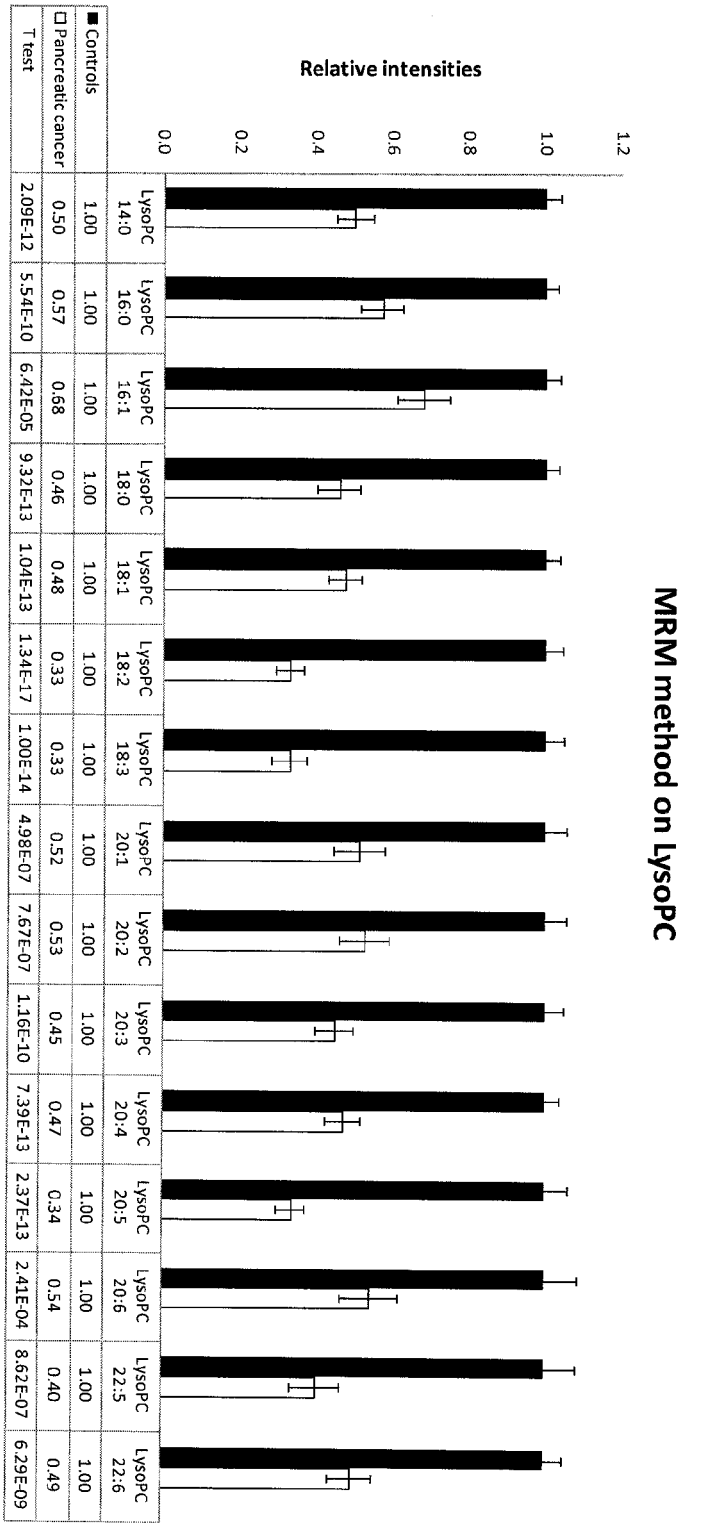
(c)



	LysoPC 30:1	LysoPC 32:0	LysoPC 32:1	LysoPC 32:2	LysoPC 32:6
■ Controls	1.00	1.00	1.00	1.00	1.00
□ Pancreatic	0.44	0.52	0.44	0.38	0.49
▩ P values	3.94E-12	1.72E-07	1.03E-11	2.81E-14	3.19E-05

Figure 41 (Cont.)

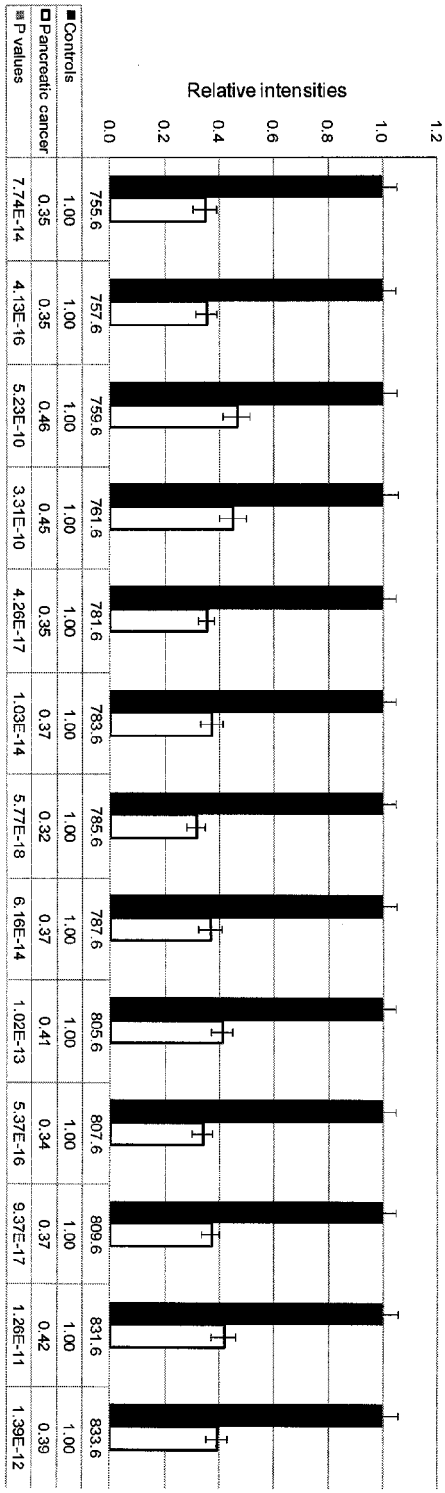
(d)



	LysoPC 14:0	LysoPC 16:0	LysoPC 16:1	LysoPC 18:0	LysoPC 18:1	LysoPC 18:2	LysoPC 18:3	LysoPC 20:1	LysoPC 20:2	LysoPC 20:3	LysoPC 20:4	LysoPC 20:5	LysoPC 20:6	LysoPC 22:5	LysoPC 22:6
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic cancer	0.50	0.57	0.68	0.46	0.48	0.33	0.33	0.52	0.53	0.45	0.47	0.34	0.54	0.40	0.49
⊤ test	2.09E-12	5.54E-10	6.42E-05	9.32E-13	1.04E-13	1.34E-17	1.00E-14	4.98E-07	7.67E-07	1.16E-10	7.39E-13	2.37E-13	2.41E-04	8.62E-07	6.29E-09

Figure 41 (Cont.)

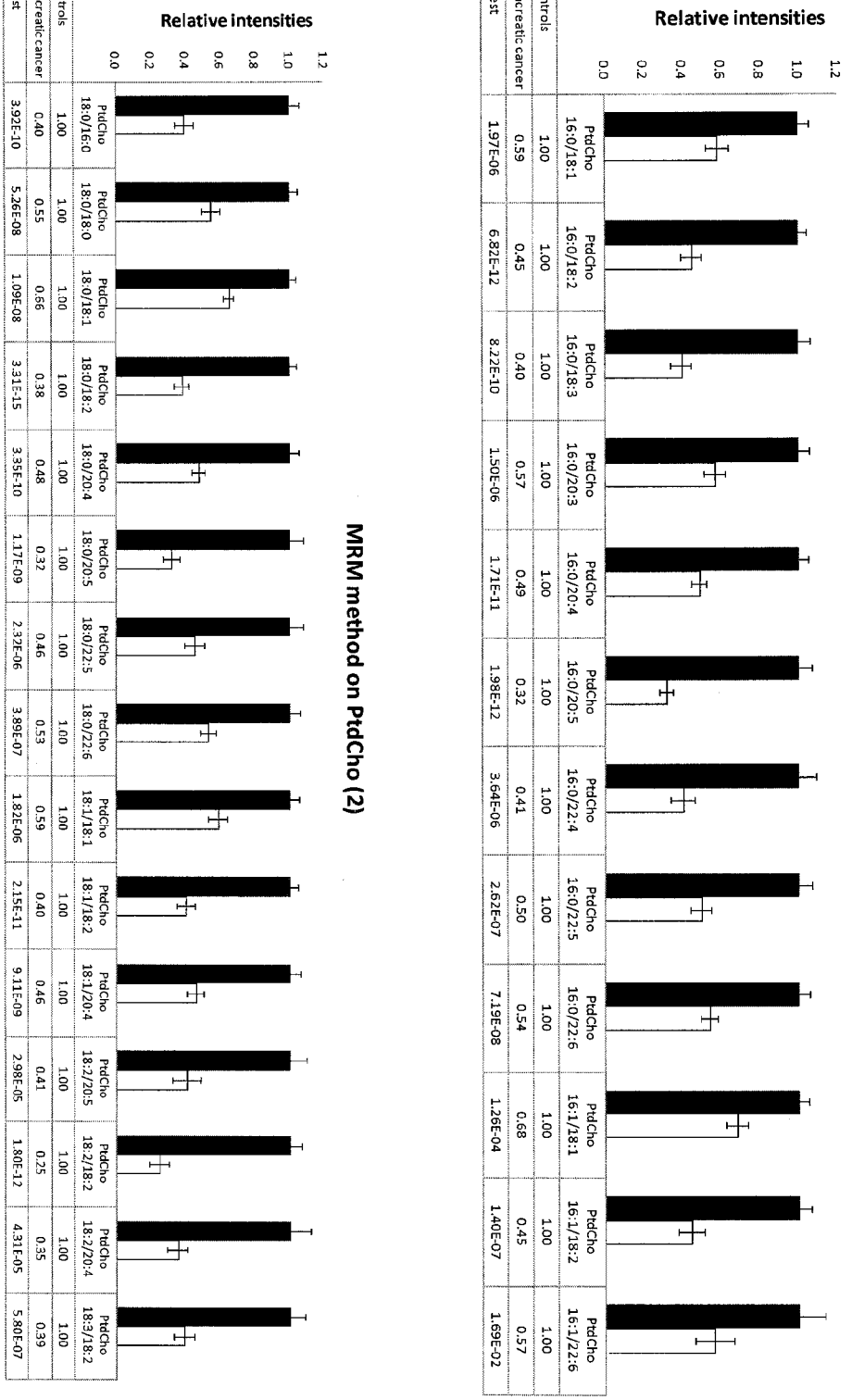
a)



	755.6	757.6	759.6	761.6	781.6	783.6	785.6	787.6	805.6	807.6	809.6	831.6	833.6
■Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□Pancreatic cancer	0.35	0.35	0.46	0.45	0.35	0.37	0.32	0.37	0.41	0.34	0.37	0.42	0.39
■P values	7.74E-14	4.13E-16	5.23E-10	3.31E-10	4.26E-17	1.03E-14	5.77E-18	6.16E-14	1.02E-13	5.37E-16	9.37E-17	1.26E-11	1.39E-12

Figure 42

b)

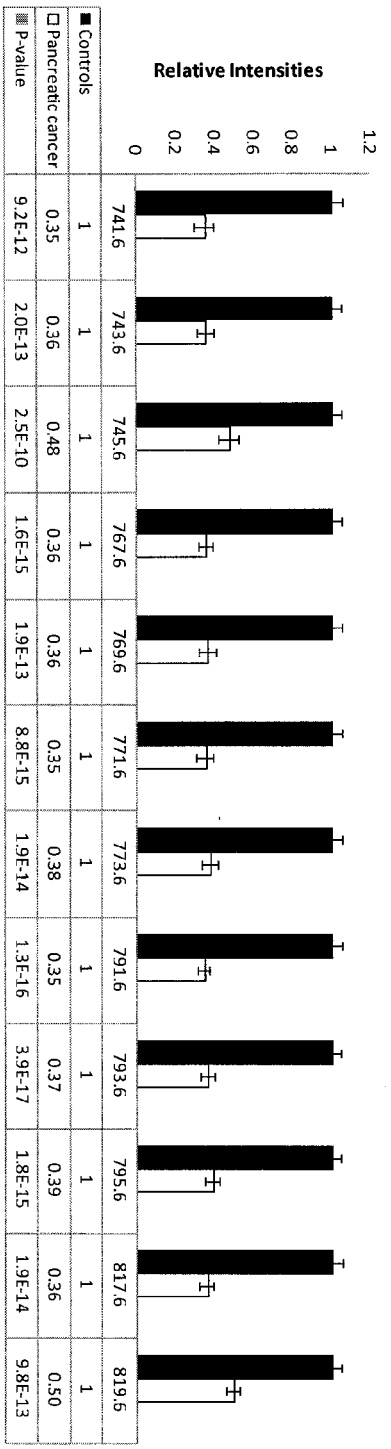


	PtdCho 16:0/18:1	PtdCho 16:0/18:2	PtdCho 16:0/18:3	PtdCho 16:0/20:3	PtdCho 16:0/20:4	PtdCho 16:0/20:5	PtdCho 16:0/22:4	PtdCho 16:0/22:5	PtdCho 16:0/22:6	PtdCho 16:1/18:1	PtdCho 16:1/18:2	PtdCho 16:1/22:6
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic cancer	0.59	0.45	0.40	0.57	0.49	0.32	0.41	0.50	0.54	0.68	0.45	0.57
T test	1.97E-06	6.82E-12	8.22E-10	1.50E-06	1.71E-11	1.98E-12	3.64E-06	2.62E-07	7.19E-08	1.26E-04	1.40E-07	1.69E-02

	PtdCho 18:0/16:0	PtdCho 18:0/18:0	PtdCho 18:0/18:1	PtdCho 18:0/18:2	PtdCho 18:0/20:4	PtdCho 18:0/20:5	PtdCho 18:0/22:5	PtdCho 18:0/22:6	PtdCho 18:1/18:1	PtdCho 18:1/18:2	PtdCho 18:1/20:4	PtdCho 18:2/20:5	PtdCho 18:2/18:2	PtdCho 18:2/20:4	PtdCho 18:3/18:2
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic cancer	0.40	0.55	0.66	0.38	0.48	0.32	0.46	0.53	0.59	0.40	0.46	0.41	0.25	0.35	0.39
T test	3.92E-10	5.26E-08	1.09E-08	3.31E-15	3.35E-10	1.17E-09	2.32E-06	3.89E-07	1.82E-06	2.15E-11	9.11E-09	2.98E-05	1.80E-12	4.31E-05	5.80E-07

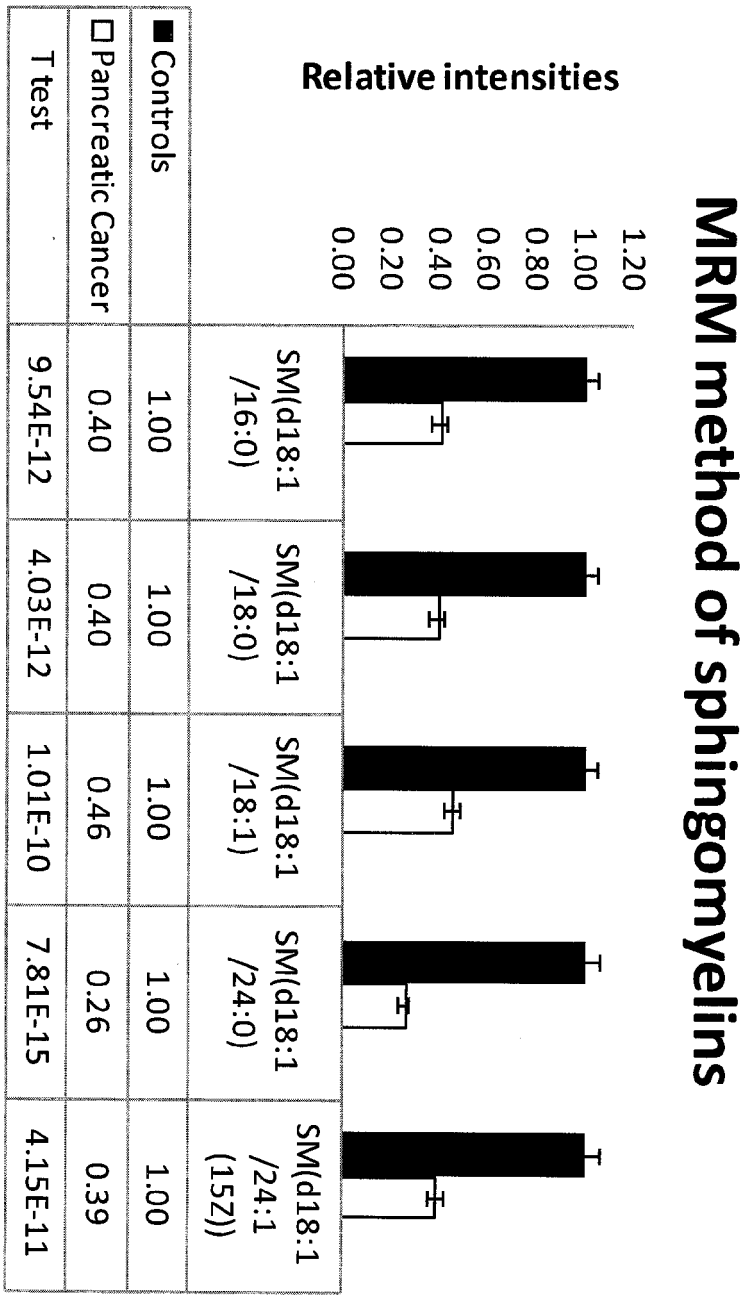
Figure 42 (cont.)

c)



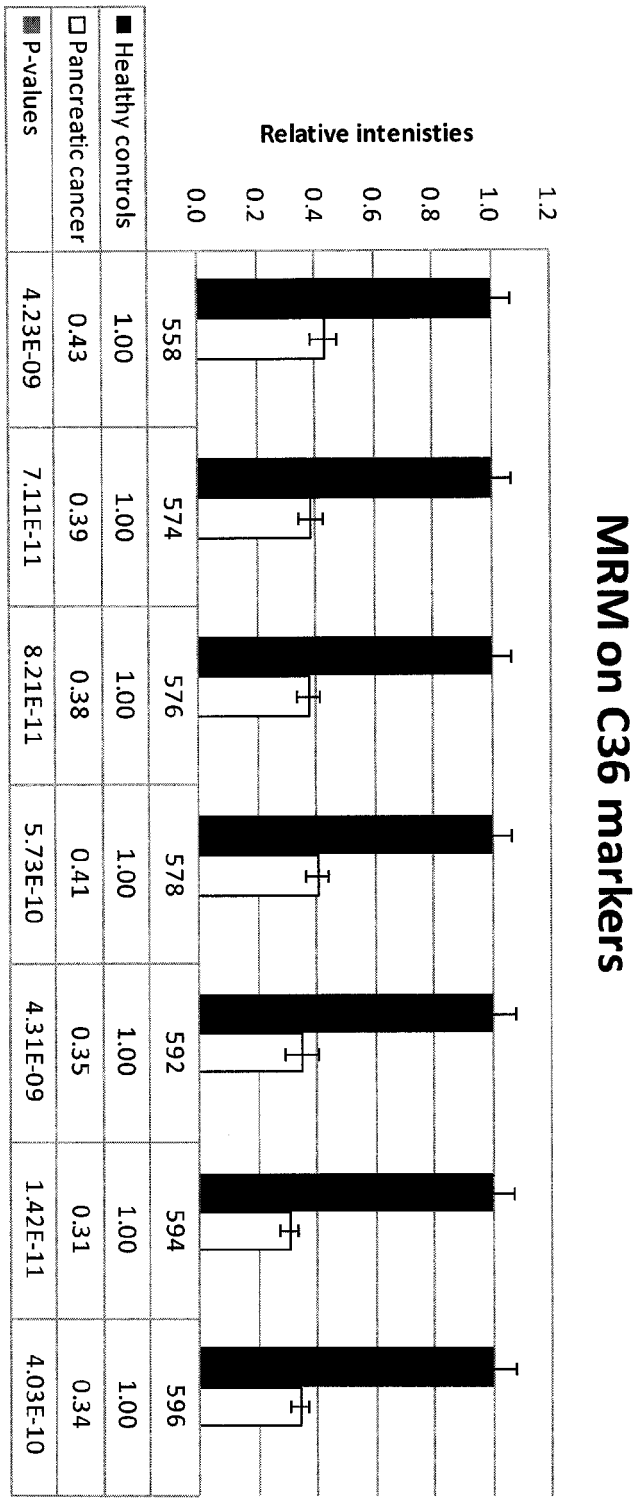
	741.6	743.6	745.6	767.6	769.6	771.6	773.6	791.6	793.6	795.6	817.6	819.6
■ Controls	1	1	1	1	1	1	1	1	1	1	1	1
□ Pancreatic cancer	0.35	0.36	0.48	0.36	0.36	0.35	0.38	0.35	0.37	0.39	0.36	0.50
▒ P-value	9.2E-12	2.0E-13	2.5E-10	1.6E-15	1.9E-13	8.8E-15	1.9E-14	1.3E-16	3.9E-17	1.8E-15	1.9E-14	9.8E-13

Figure 42 (Cont.)



	SM(d18:1/16:0)	SM(d18:1/18:0)	SM(d18:1/18:1)	SM(d18:1/24:0)	SM(d18:1/24:1(15Z))
■ Controls	1.00	1.00	1.00	1.00	1.00
□ Pancreatic Cancer	0.40	0.40	0.46	0.26	0.39
T test	9.54E-12	4.03E-12	1.01E-10	7.81E-15	4.15E-11

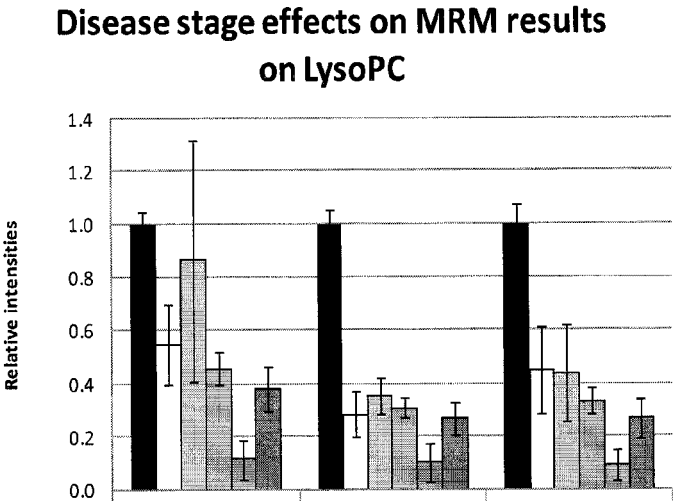
Figure 43



	558	574	576	578	592	594	596
■ Healthy controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic cancer	0.43	0.39	0.38	0.41	0.35	0.31	0.34
■ P-values	4.23E-09	7.11E-11	8.21E-11	5.73E-10	4.31E-09	1.42E-11	4.03E-10

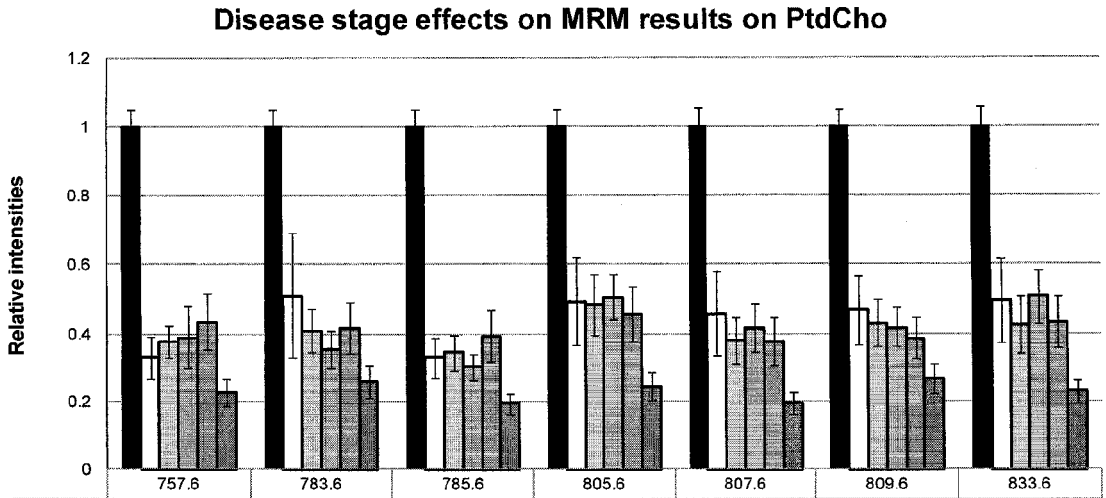
Figure 44

(a)



	LysoCh 18:0	LysoCh 18:2	LysoCh 20:5
Controls	1.00	1.00	1.00
Stage I	0.54	0.28	0.45
Stage II	0.86	0.35	0.44
Stage III	0.46	0.31	0.33
Stage IVa	0.11	0.10	0.09
Stage IVb	0.38	0.27	0.27

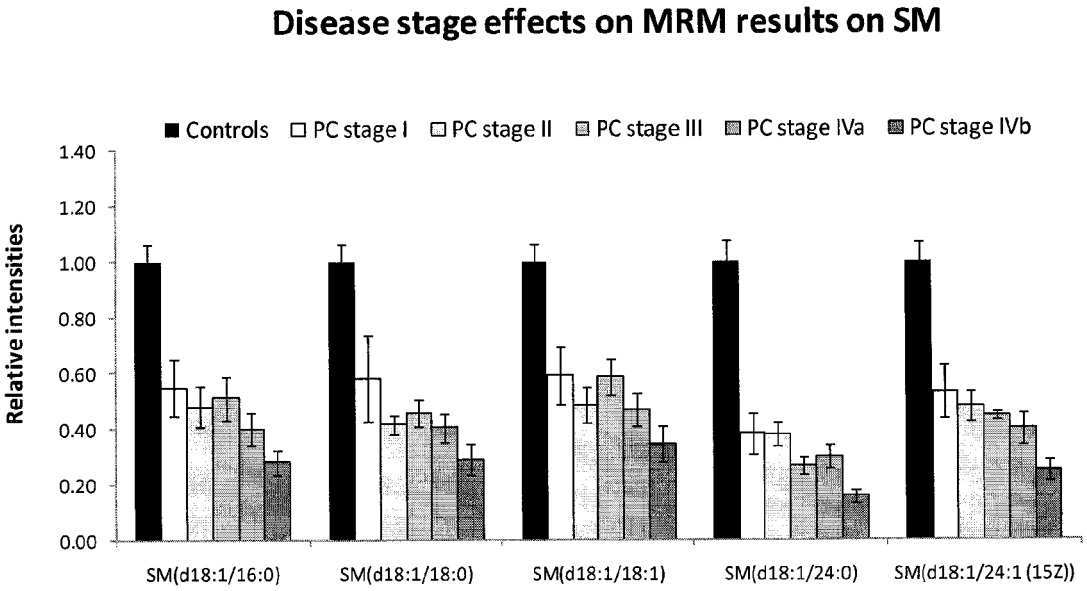
(b)



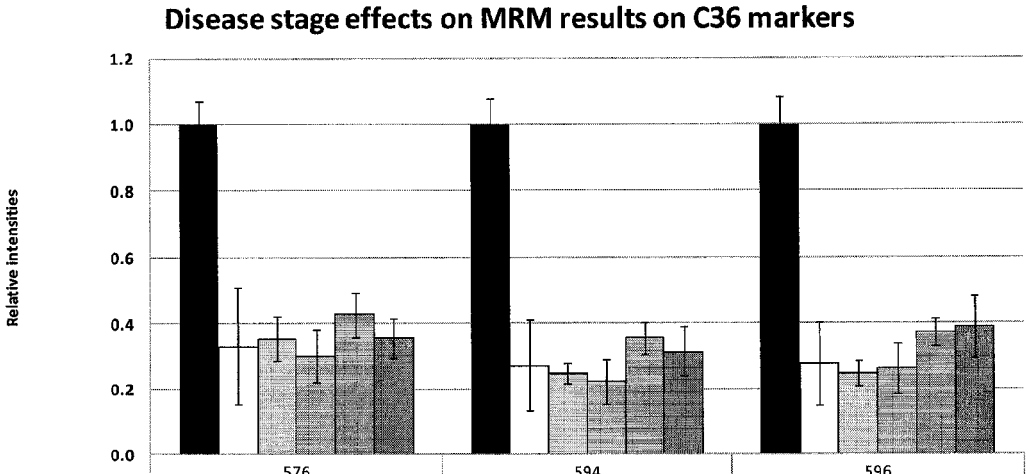
	757.6	783.6	785.6	805.6	807.6	809.6	833.6
Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Stage I	0.33	0.51	0.33	0.49	0.46	0.47	0.50
Stage II	0.38	0.41	0.34	0.48	0.38	0.43	0.43
Stage III	0.39	0.35	0.30	0.51	0.42	0.42	0.51
Stage IVa	0.43	0.42	0.39	0.46	0.38	0.39	0.43
Stage IVb	0.22	0.26	0.19	0.24	0.19	0.27	0.23

Figure 45

(c)



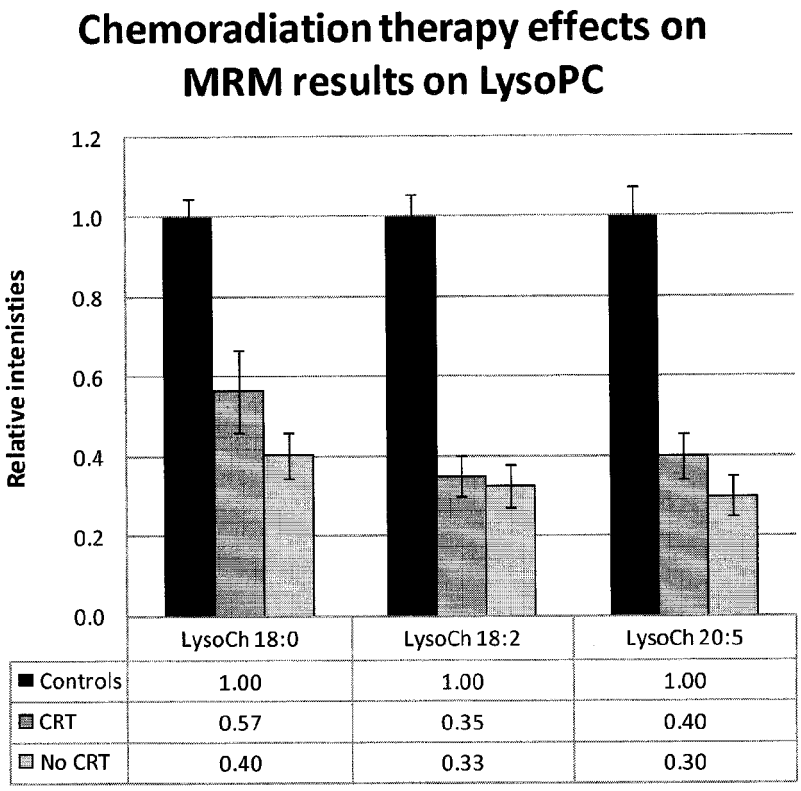
(d)



	576	594	596
Healthy controls	1.00	1.00	1.00
Stage I	0.33	0.27	0.28
Stage II	0.36	0.25	0.25
Stage III	0.30	0.22	0.26
Stage IVa	0.43	0.36	0.37
Stage IVb	0.36	0.31	0.39

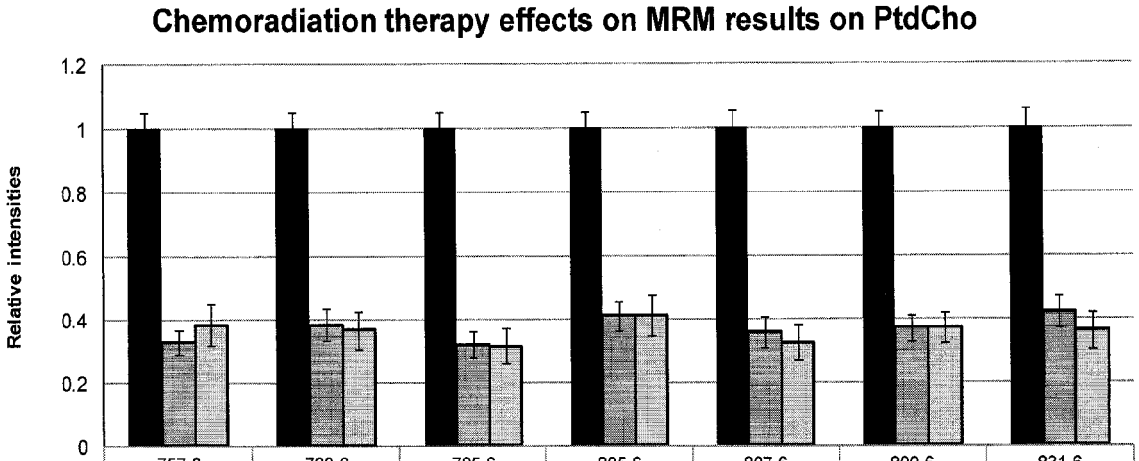
Figure 45 (Cont.)

(a)



	LysoCh 18:0	LysoCh 18:2	LysoCh 20:5
Controls	1.00	1.00	1.00
CRT	0.57	0.35	0.40
No CRT	0.40	0.33	0.30

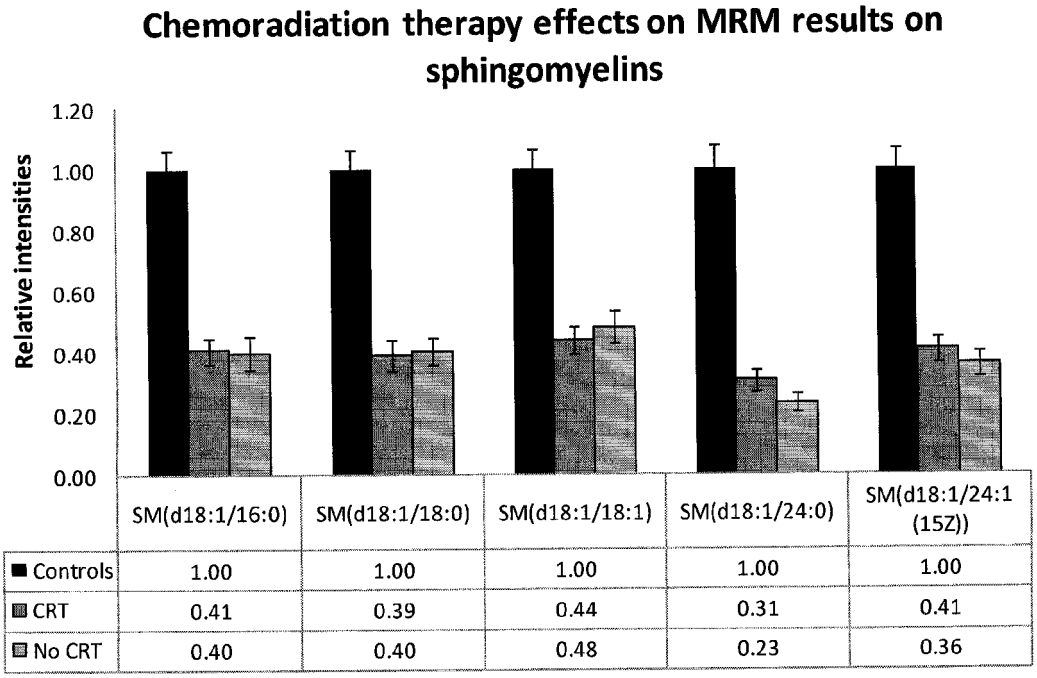
(b)



	757.6	783.6	785.6	805.6	807.6	809.6	831.6
Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00
CRT	0.33	0.38	0.32	0.41	0.36	0.37	0.42
No CRT	0.38	0.36	0.31	0.41	0.32	0.37	0.36

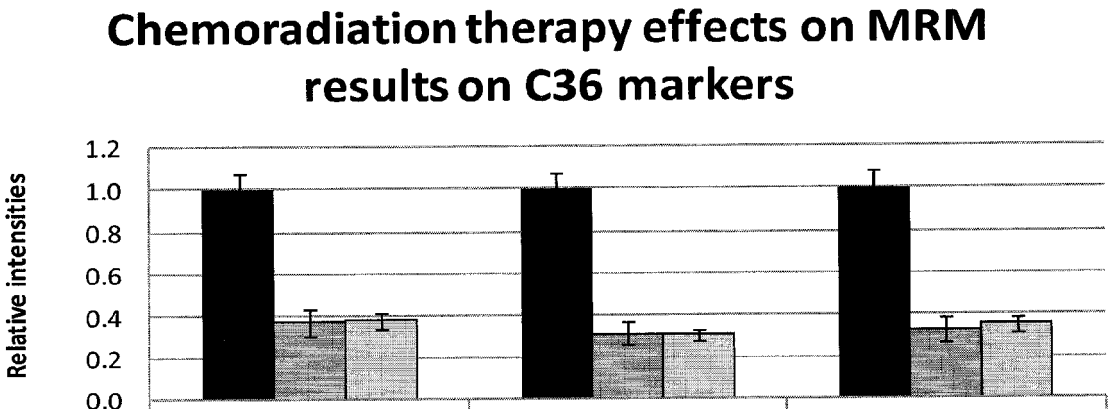
Figure 46

(c)



	SM(d18:1/16:0)	SM(d18:1/18:0)	SM(d18:1/18:1)	SM(d18:1/24:0)	SM(d18:1/24:1 (15Z))
Controls	1.00	1.00	1.00	1.00	1.00
CRT	0.41	0.39	0.44	0.31	0.41
No CRT	0.40	0.40	0.48	0.23	0.36

(d)



	576	594	596
Controls	1.00	1.00	1.00
CRT	0.37	0.31	0.33
No CRT	0.38	0.31	0.35

Figure 46 (Cont.)