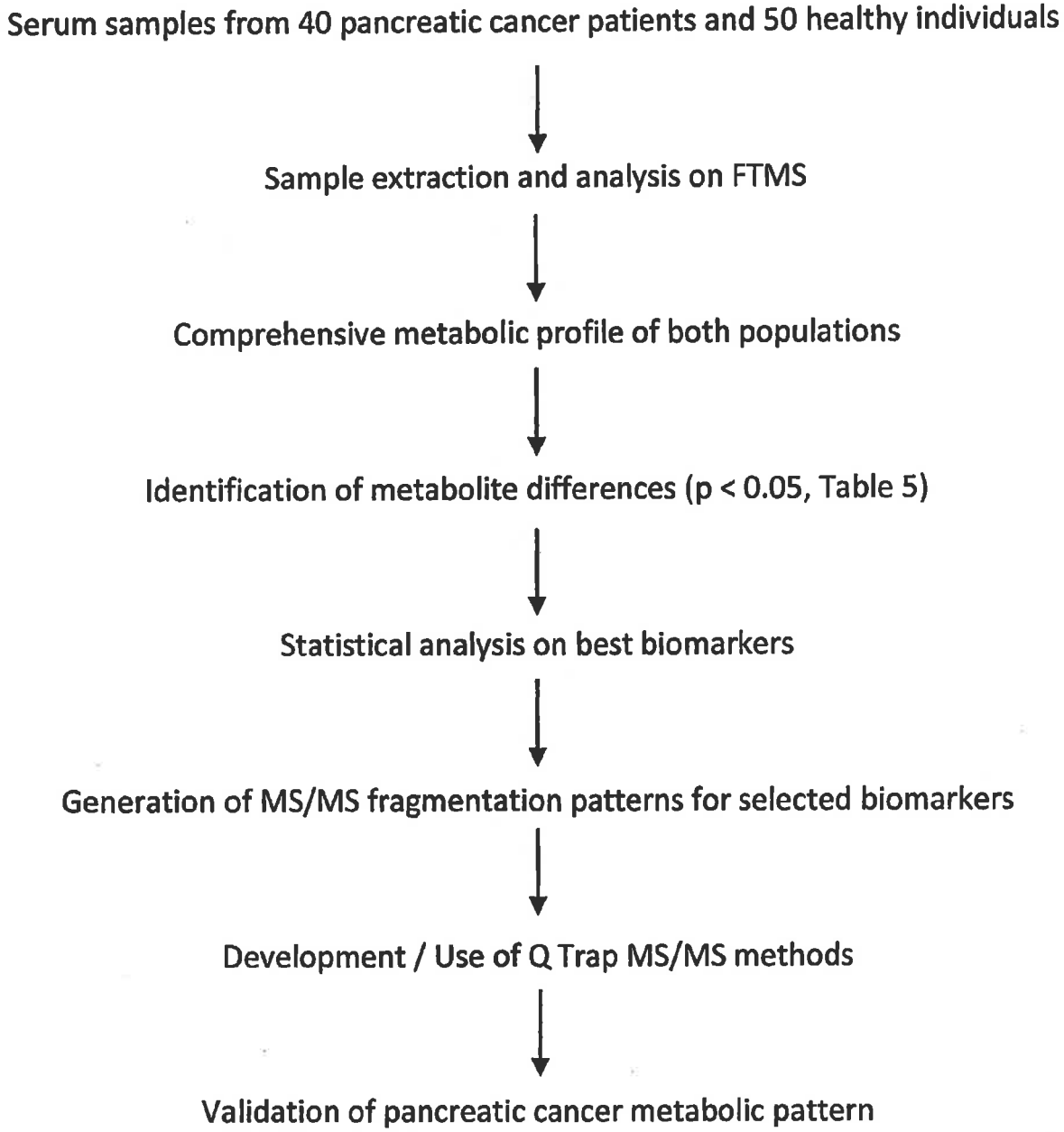

Serum samples from 40 pancreatic cancer patients and 50 healthy individuals
Sample extraction and analysis on FTMS
Comprehensive metabolic profile of both populations
Identification of metabolite differences (p < 0.05, Table 5)
Statistical analysis on best biomarkers
Generation of MS/MS fragmentation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

Figure 1

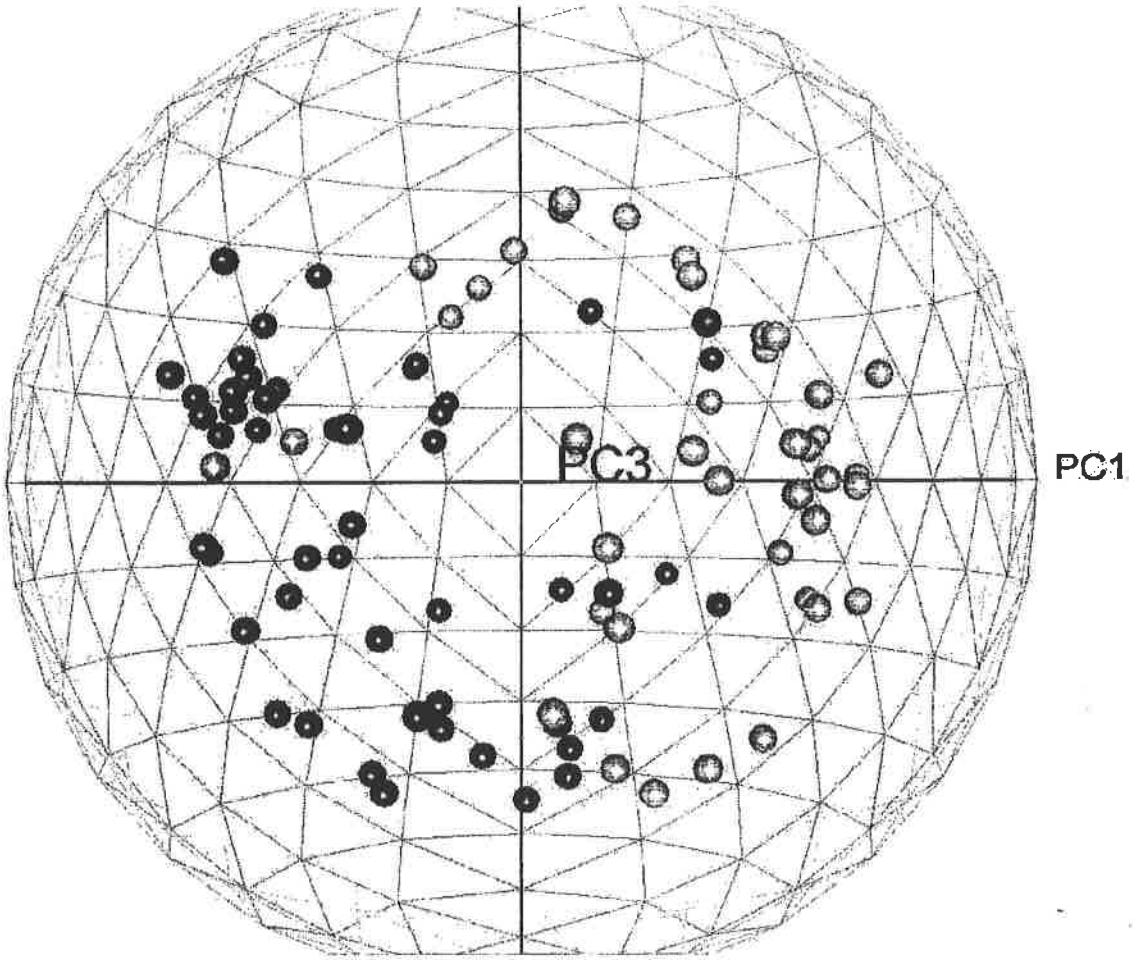


Figure 2

a)

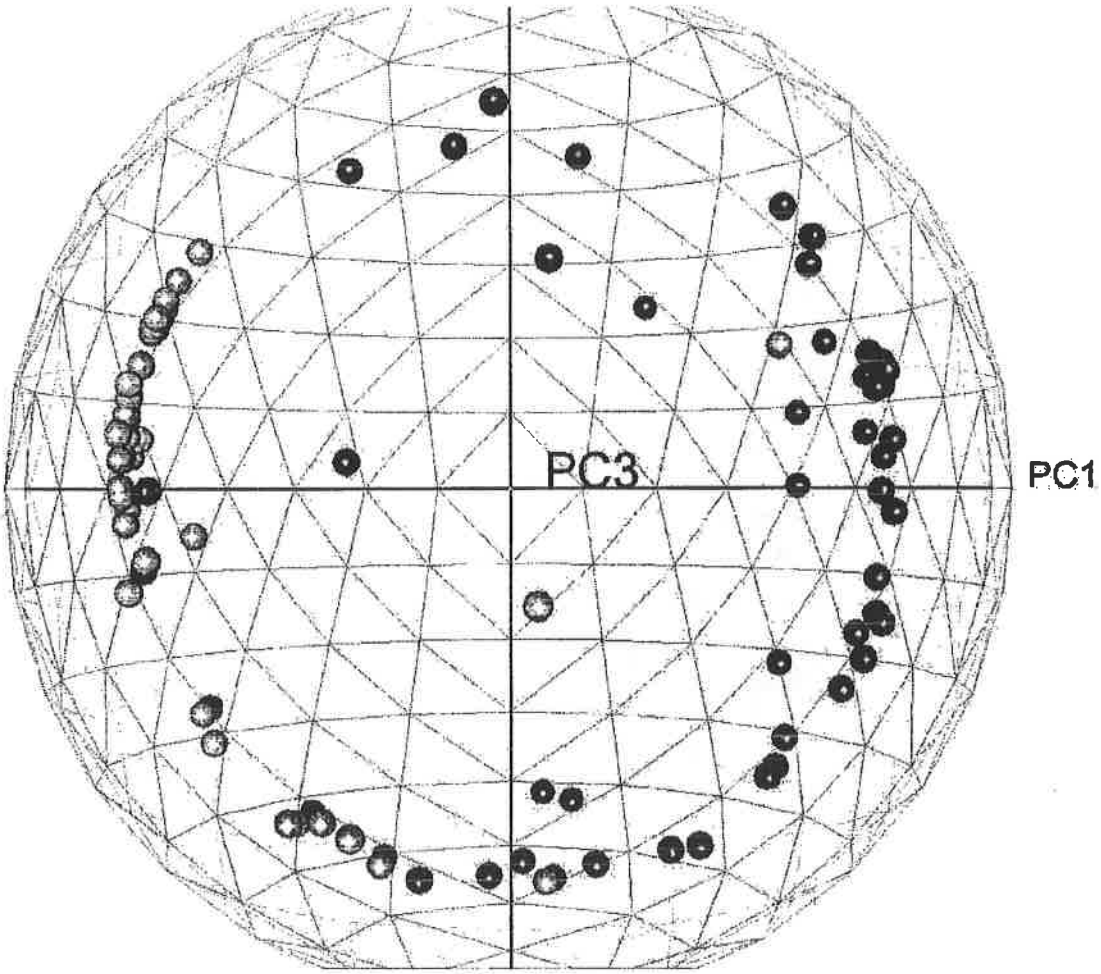
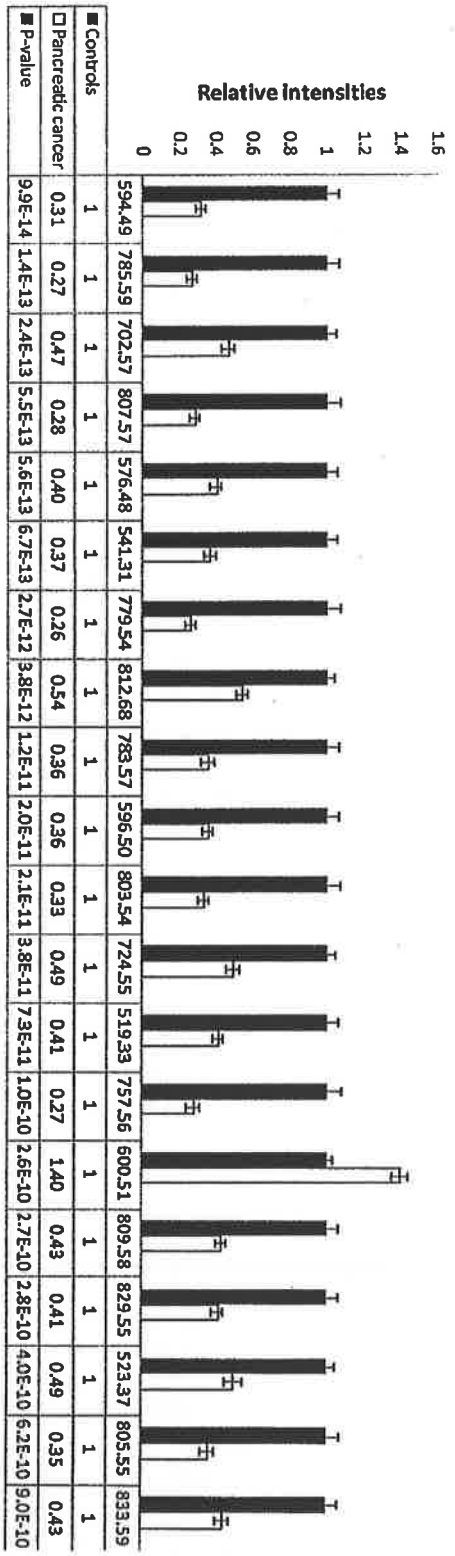


Figure 3

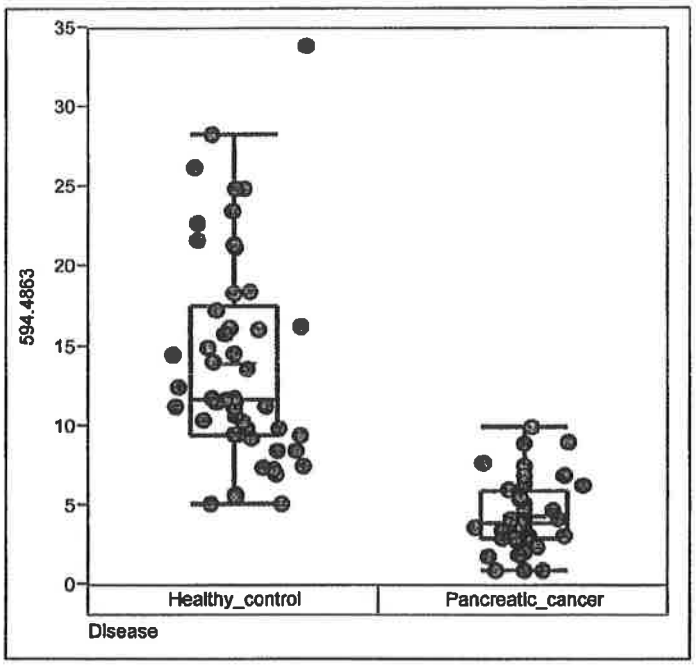
b)



	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

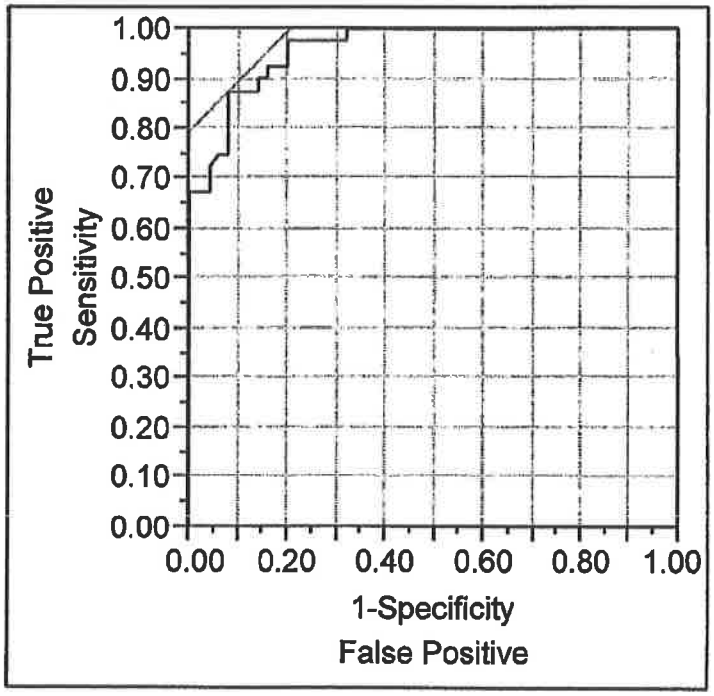
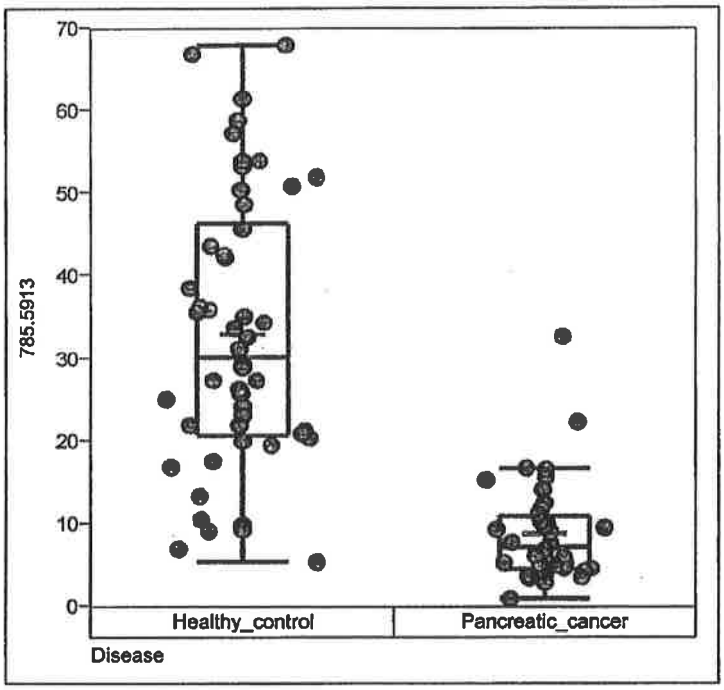

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
True Positive
Sensitivity
0.00
0.20
0.40
0.60
0.80
1.00
1-Specificity
False Positive

Figure 4

(b)



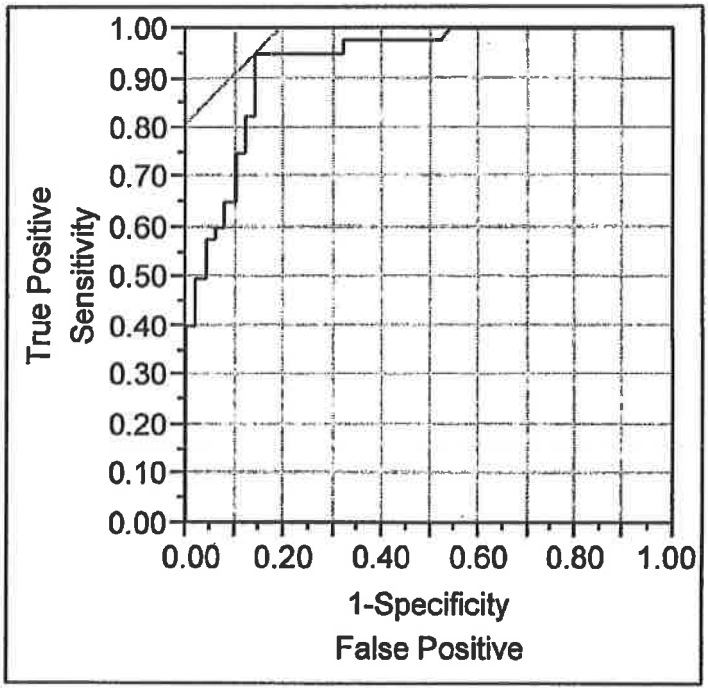
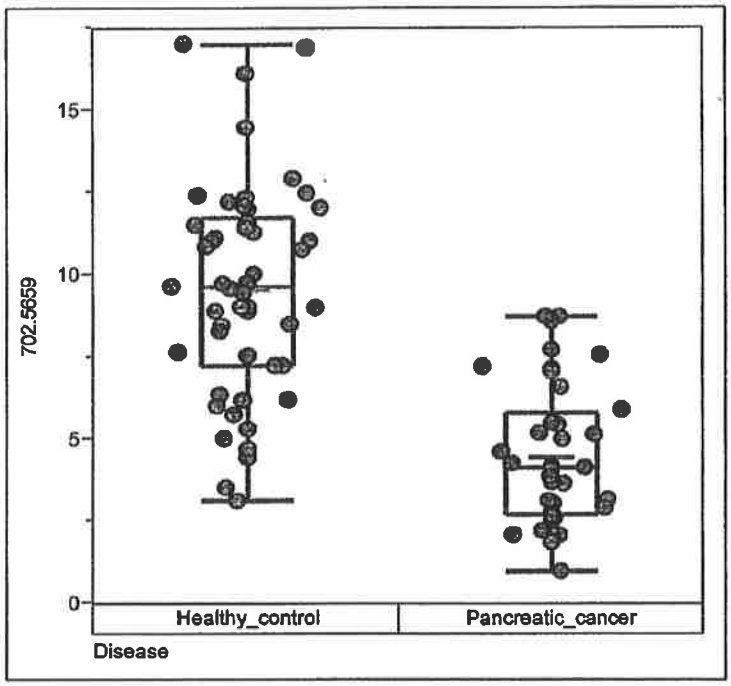


Figure 4 (cont.)

(c)



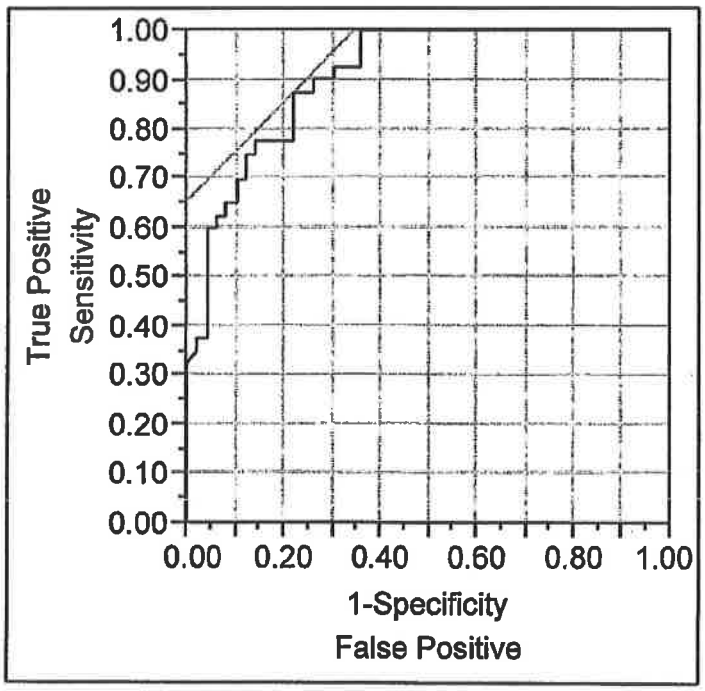
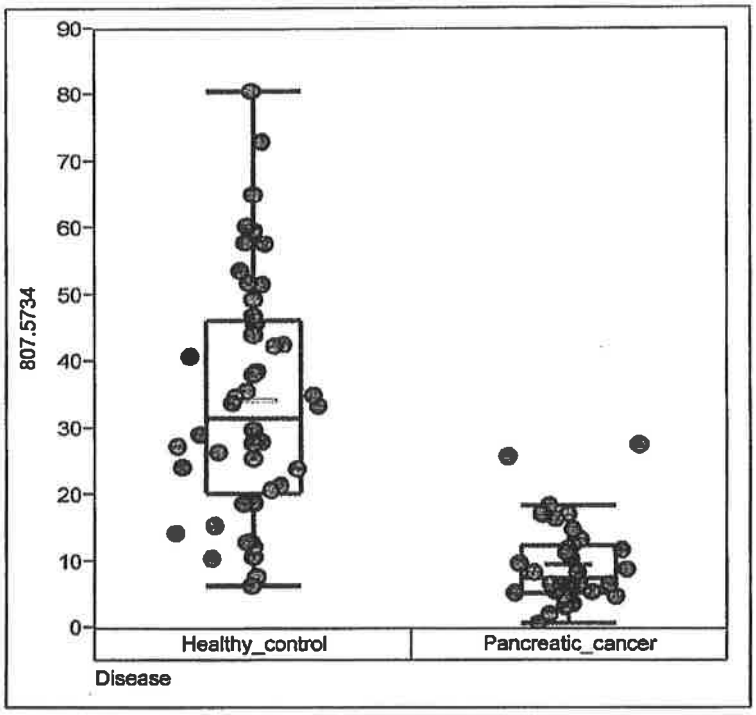


Figure 4 (cont.)

(d)



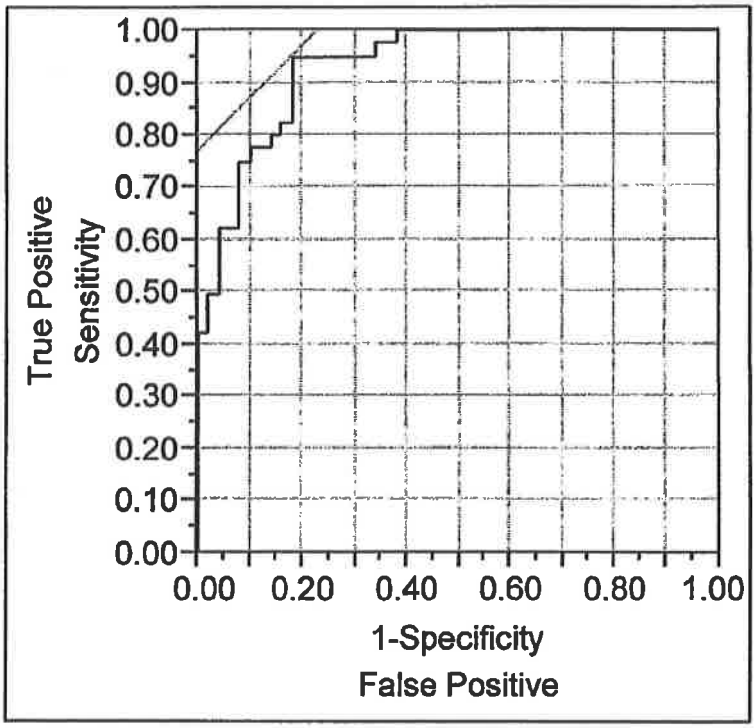
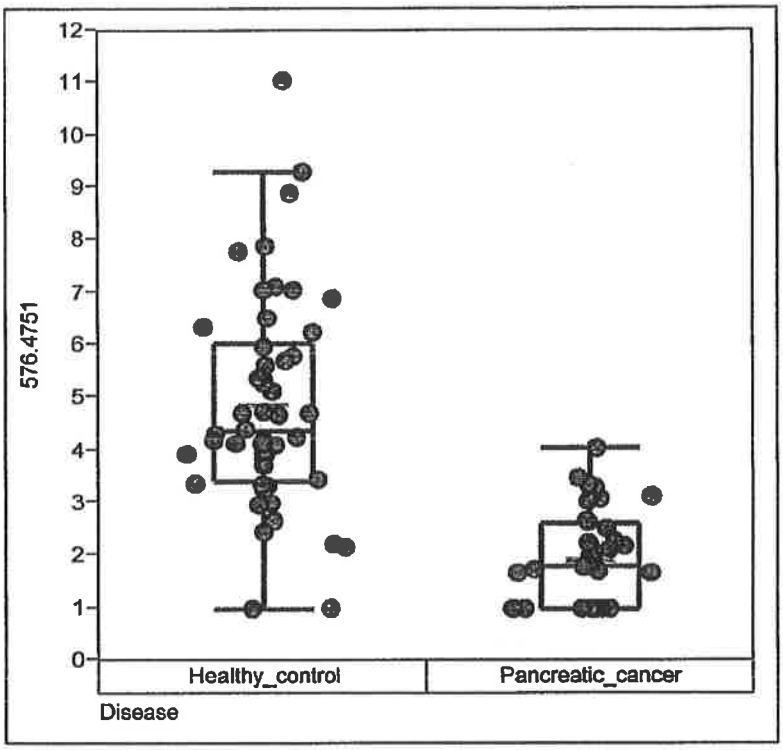


Figure 4 (cont.)

(e)



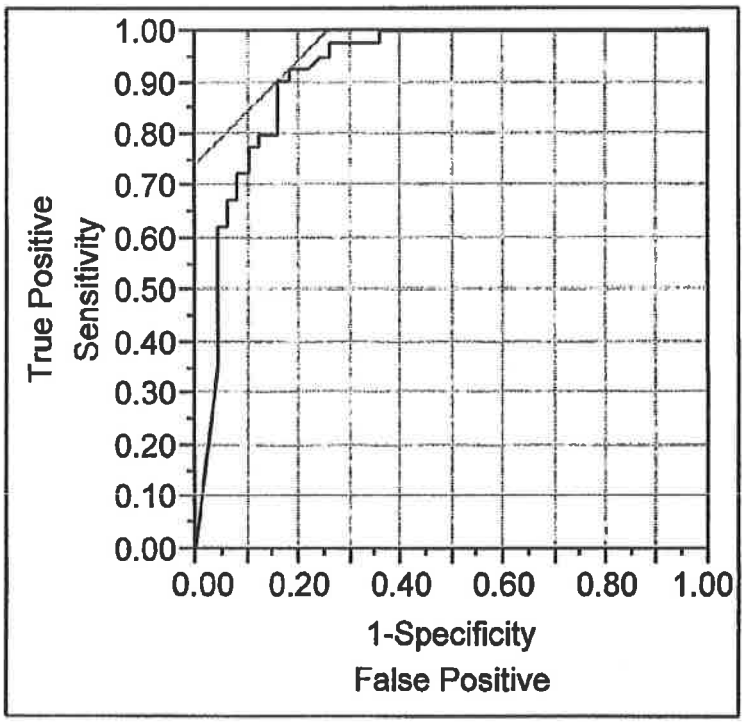
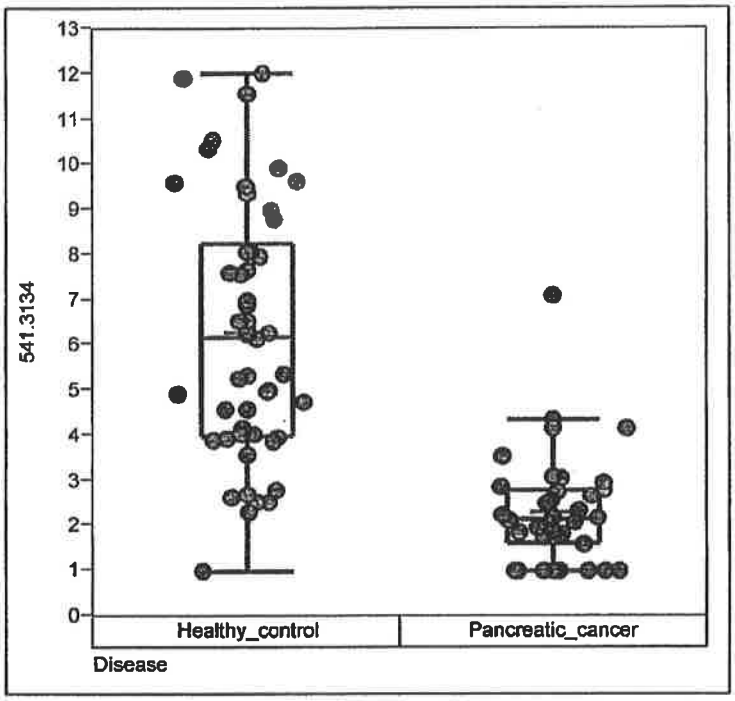


Figure 4 (cont.)

(f)



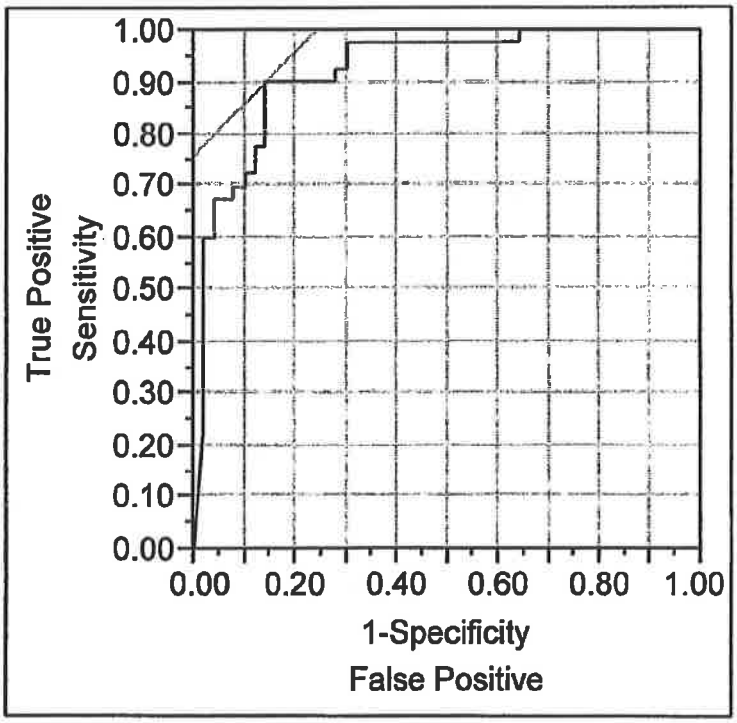
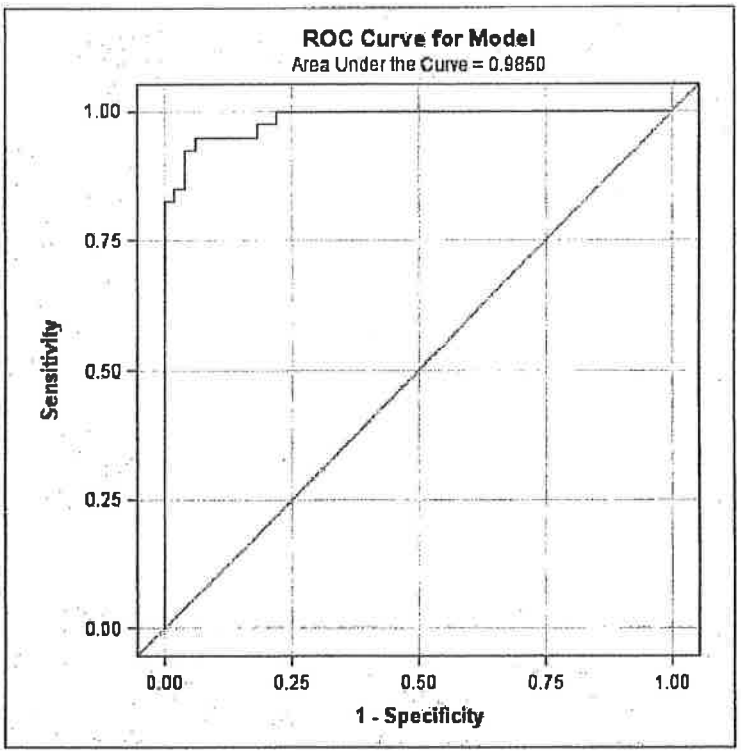


Figure 4 (cont.)

(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

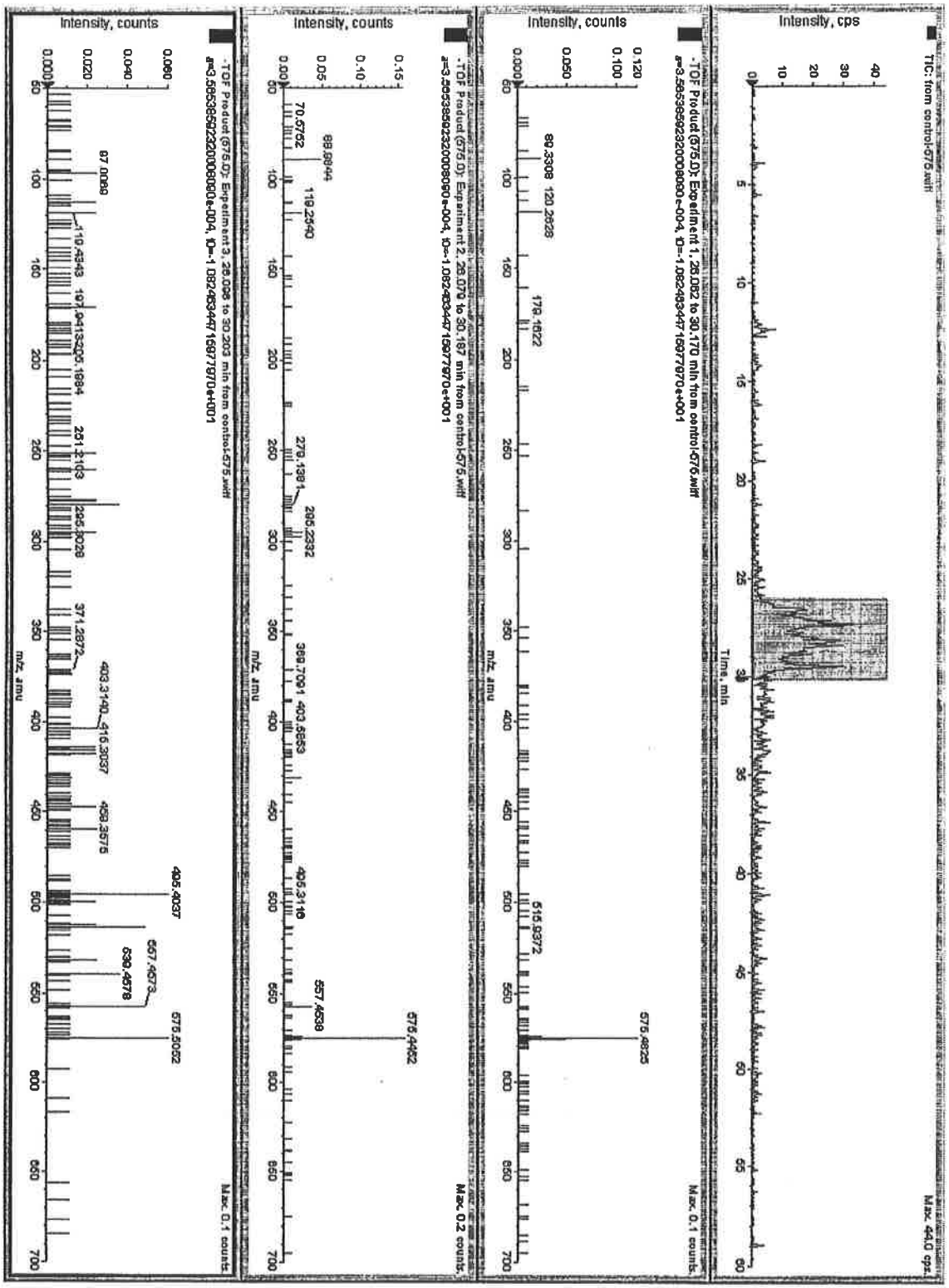

TIC: from control-575.wiff
Intensity, cps
Max. 44.0 cps.
Time, min
-TOF Product (575.0): Experiment 1, 26.082 to 30.170 min from control-575.wiff
Intensity, counts
Max. 0.1 counts.
m/z, amu
-TOF Product (575.0): Experiment 2, 26.079 to 30.197 min from control-575.wiff
Max. 0.2 counts.
-TOF Product (575.0): Experiment 3, 26.098 to 30.203 min from control-575.wiff
Max. 0.1 counts.

Figure 6

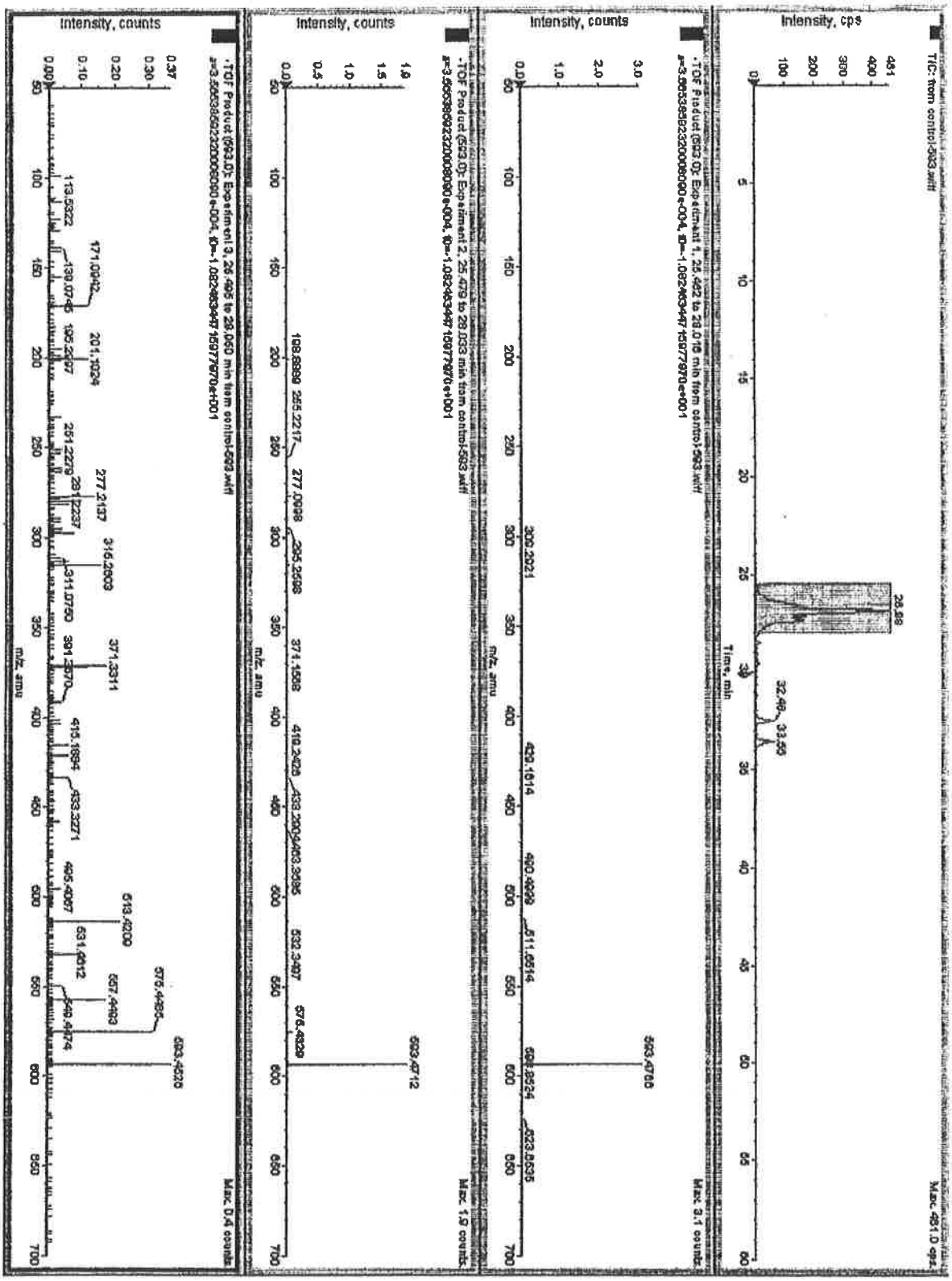

TIC: from control-593.wiff
Intensity, cps
Time, min
Max. 481.0 cps.
-TOF Product (593.0): Experiment 1, 25.462 to 28.016 min from control-593.wiff
Intensity, counts
m/z, amu
Max. 3.1 counts.
-TOF Product (593.0): Experiment 2, 25.479 to 28.033 min from control-593.wiff
Max. 1.9 counts.
-TOF Product (593.0): Experiment 3, 24.495 to 28.050 min from control-593.wiff
Max. 0.4 counts.

Figure 7

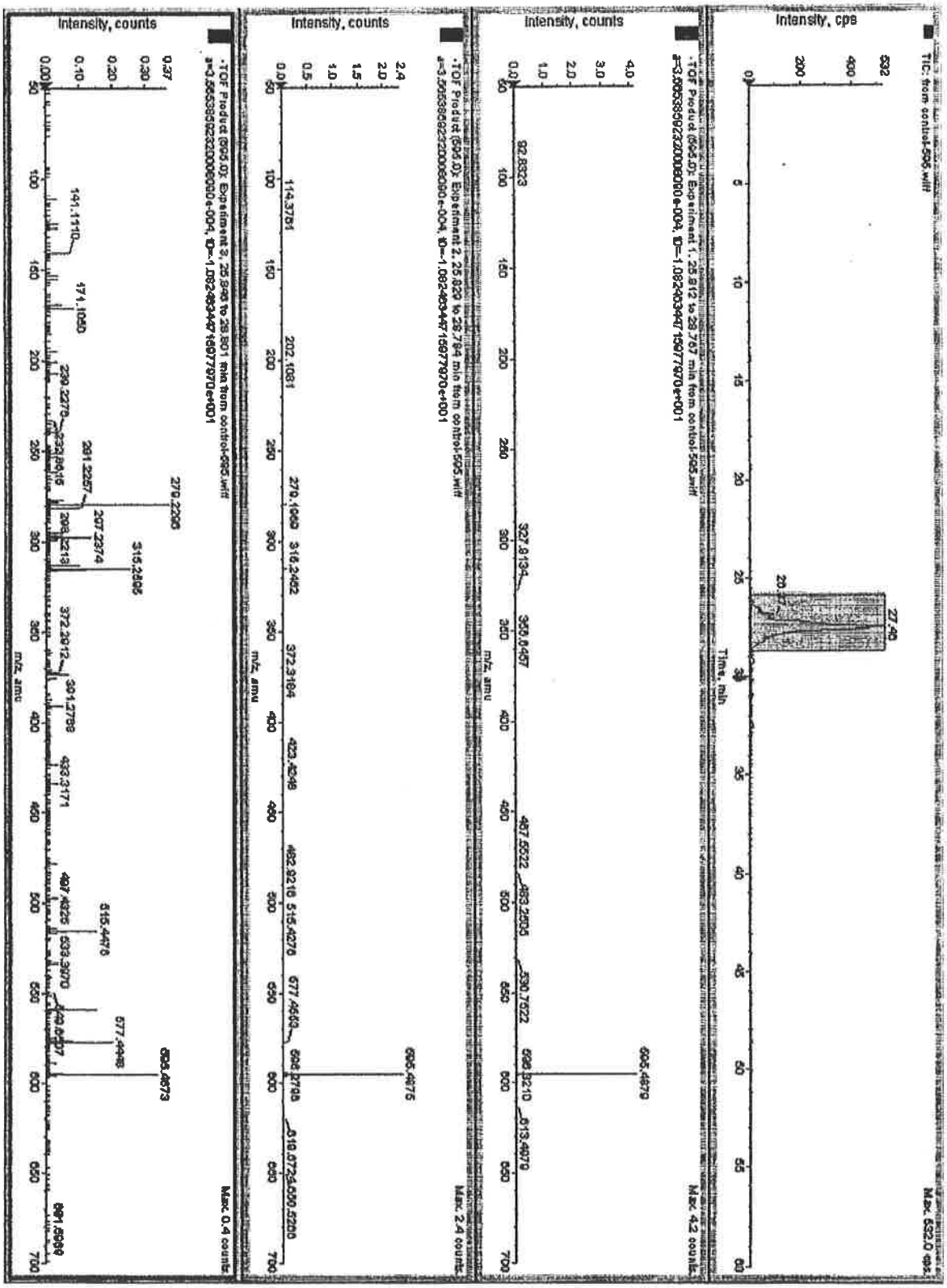

TIC: from control-595.wiff
Intensity, cps
Time, min
27.49
Max. 532.0 cps.
-TOF Product (595.0): Experiment 1, 25.812 to 28.787 min from control-595.wiff
Intensity, counts
m/z, amu
92.8323
927.8134
355.0457
487.5522
483.2605
530.7522
595.4879
698.3210
613.4079
Max. 4.2 counts.
-TOF Product (595.0): Experiment 2, 25.829 to 28.784 min from control-595.wiff
Intensity, counts
m/z, amu
114.3781
202.1081
279.1969
316.2462
372.3164
423.4048
482.9216
515.4270
677.4560
595.4875
Max. 2.4 counts.
-TOF Product (595.0): Experiment 3, 25.848 to 28.801 min from control-595.wiff
Intensity, counts
m/z, amu
141.1110
171.1050
239.2278
291.2257
297.2374
315.2595
372.2912
301.2789
433.3171
487.4025
515.4478
633.3970
577.4448
595.4673
Max. 0.4 counts.

Figure 8

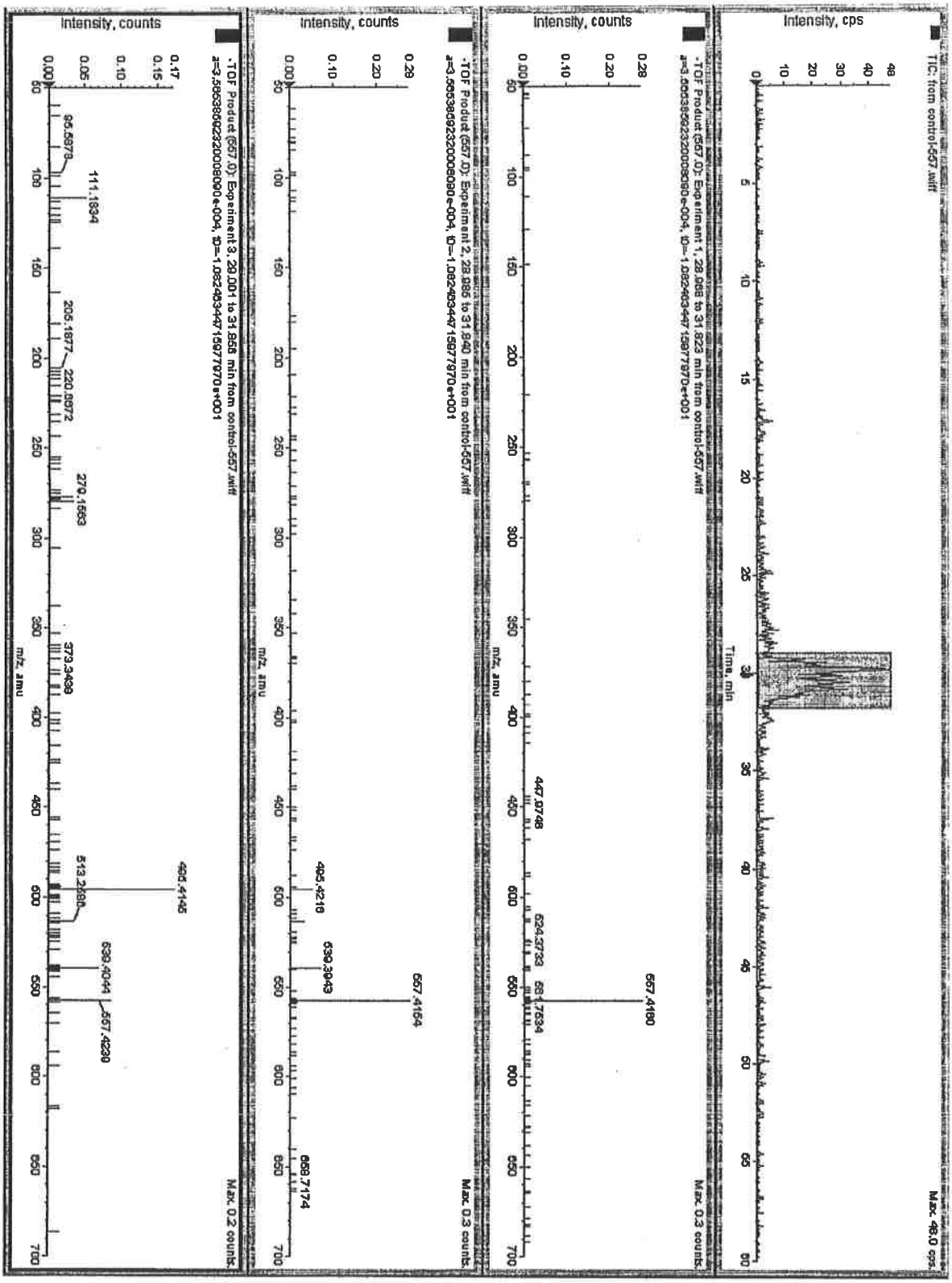

TIC: from control-557.wiff
Intensity, cps
Time, min
Max. 48.0 cps.
-TOF Product (557.0): Experiment 1, 28.668 to 31.823 min from control-557.wiff
Intensity, counts
m/z, amu
Max. 0.3 counts.
557.4160
447.9748
624.3733
681.7834
-TOF Product (557.0): Experiment 2, 28.885 to 31.940 min from control-557.wiff
557.4154
495.4216
539.3943
668.7174
-TOF Product (557.0): Experiment 3, 29.001 to 31.858 min from control-557.wiff
Max. 0.2 counts.
484.4145
513.2998
539.4044
557.4230
95.5979
111.1834
205.1677
220.9572
279.1553
373.3439

Figure 9

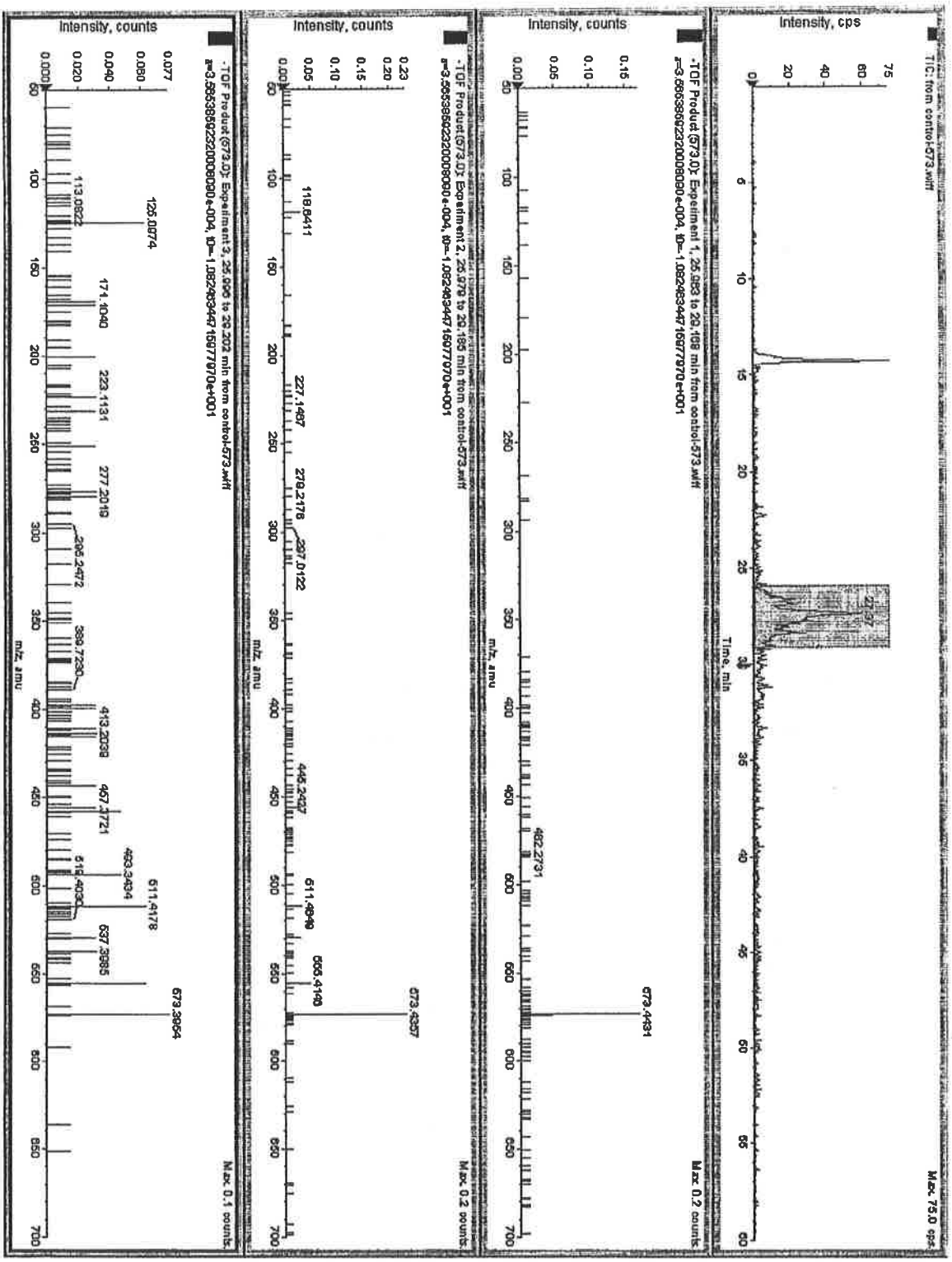

TIC: from control-573.wiff
Max 75.0 cps
Intensity, cps
Time, min
22.97
-TOF Product (573.0): Experiment 1, 25.983 to 29.168 min from control-573.wiff
z=3.55638592322000800e-004, to=-1.08249344716977970e+001
Max 0.2 counts.
Intensity, counts
m/z, amu
492.2731
573.4431
-TOF Product (573.0): Experiment 2, 29.979 to 33.185 min from control-573.wiff
z=3.55638592322000800e-004, to=-1.08249344716977970e+001
Max 0.2 counts.
Intensity, counts
m/z, amu
118.8411
227.1497
278.2178
297.0122
445.2497
511.4848
555.4148
573.4357
-TOF Product (573.0): Experiment 3, 25.696 to 29.202 min from control-573.wiff
z=3.55638592322000800e-004, to=-1.08249344716977970e+001
Max. 0.1 counts.
Intensity, counts
m/z, amu
125.0774
113.0822
171.1040
223.1131
277.2019
295.2472
389.7230
413.2038
457.3721
463.3434
511.4178
537.3985
573.3954

Figure 10

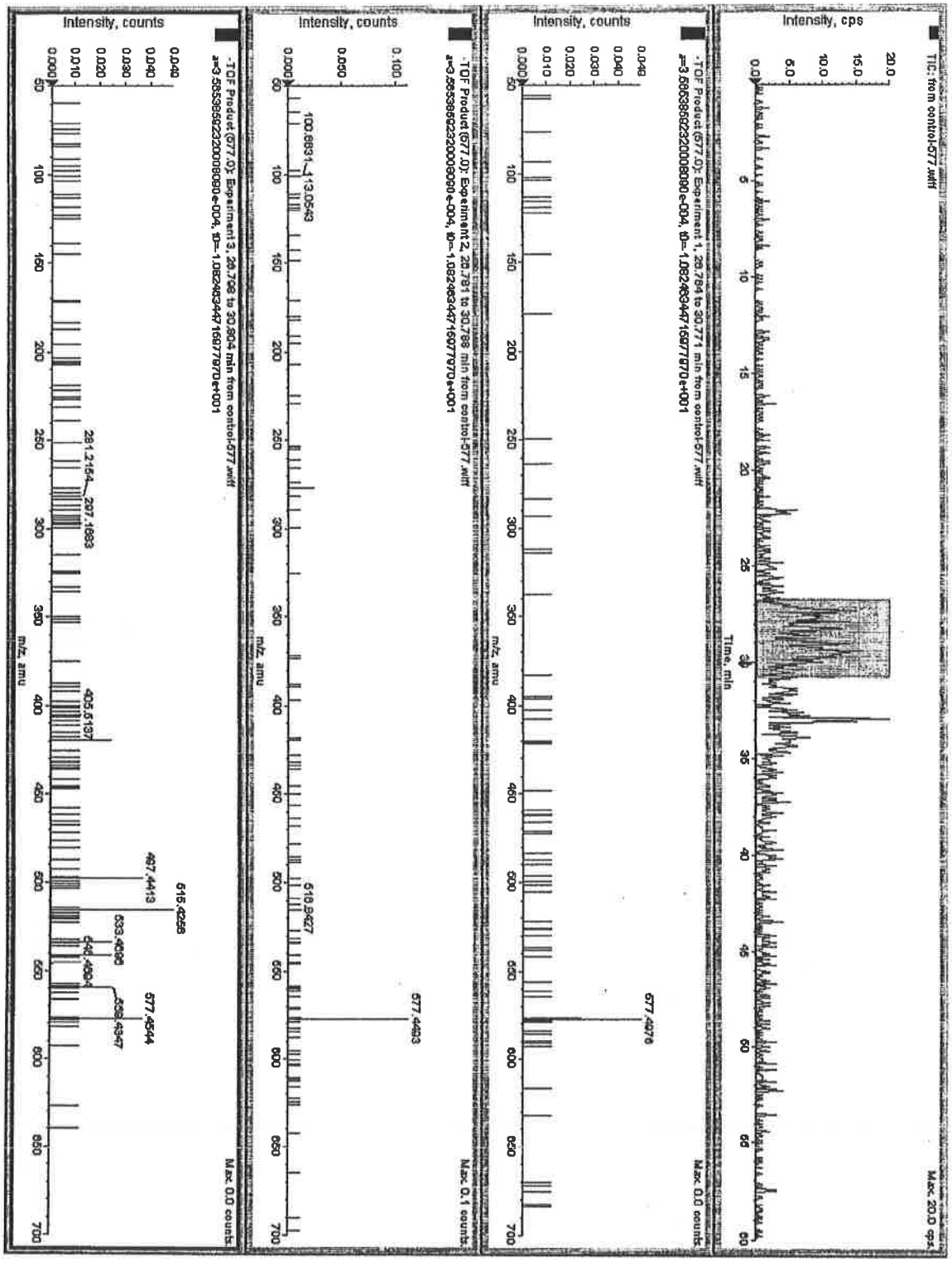

TIC: from control-577.wiff
Max. 20.0 cps.
Intensity, cps
Time, min
- TOF Product (577.0): Experiment 1, 28.784 to 30.771 min from control-577.wiff
a=3.58536852320006090e-004, t0=-1.08246344716977670e+001
Max. 0.0 counts.
Intensity, counts
m/z, amu
577.4976
- TOF Product (577.0): Experiment 2, 28.791 to 30.798 min from control-577.wiff
a=3.58536852320006090e-004, t0=-1.08246344716977670e+001
Max. 0.1 counts.
100.6691
113.0543
519.5427
577.4493
- TOF Product (577.0): Experiment 3, 28.798 to 30.804 min from control-577.wiff
a=3.58536852320006090e-004, t0=-1.08246344716977670e+001
Max. 0.0 counts.
281.2154
297.1683
405.5137
497.4419
515.4255
533.4595
546.4904
558.4347
577.4544

Figure 11

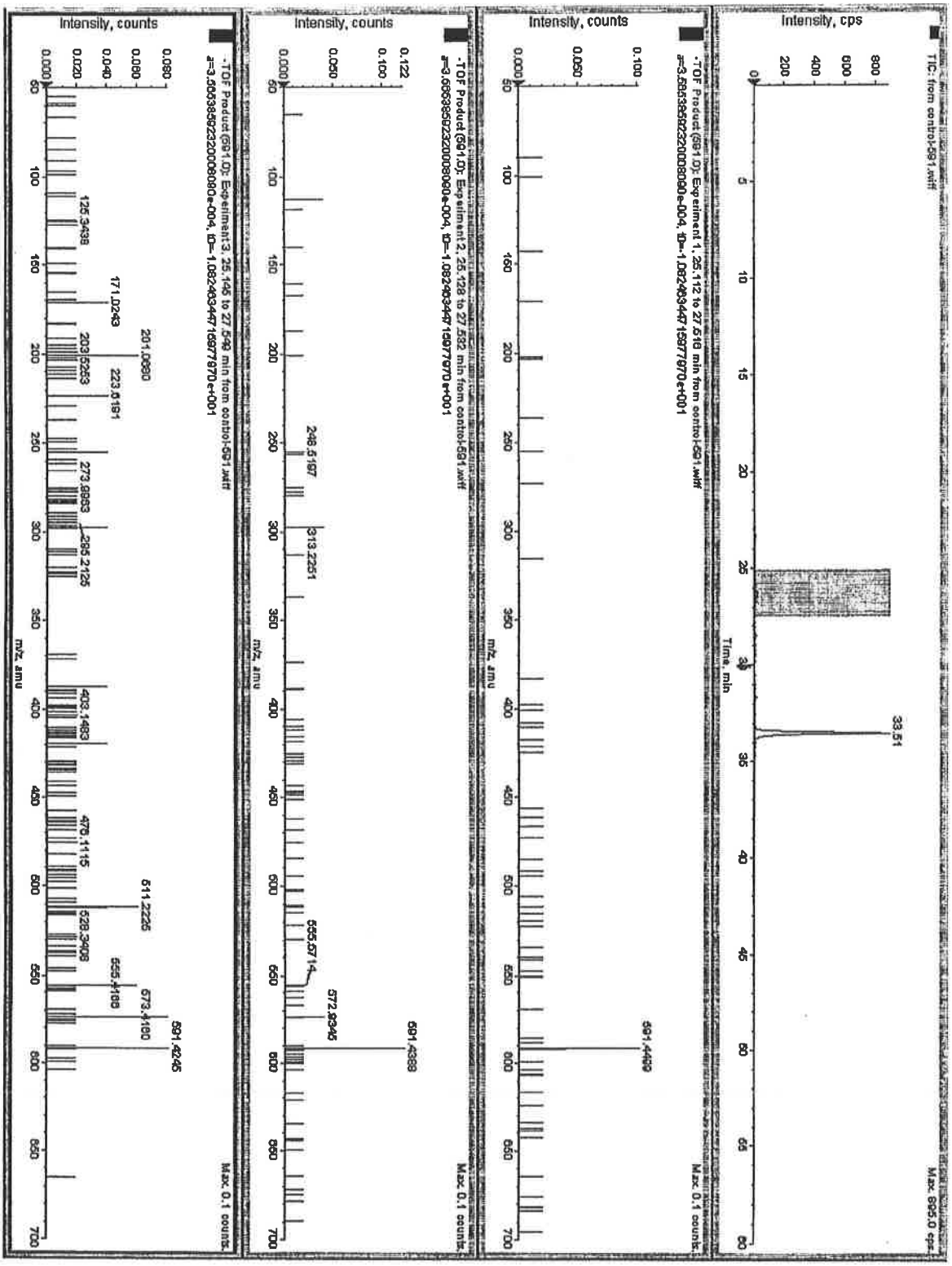

TIC: from control-591.wiff
Intensity, cps
Max. 695.0 cps.
33.51
Time, min
-TOF Product (591.0): Experiment 1, 25.112 to 27.516 min from control-591.wiff
Intensity, counts
591.4469
m/z, amu
Max. 0.1 counts.
-TOF Product (591.0): Experiment 2, 25.128 to 27.532 min from control-591.wiff
248.5167
313.2251
555.5714
572.9345
591.4369
-TOF Product (591.0): Experiment 3, 25.146 to 27.549 min from control-591.wiff
125.3438
171.0243
201.0660
203.5263
223.5191
279.9963
285.2125
403.1483
476.1115
511.2225
528.3408
555.4188
573.4190
591.4245

Figure 12

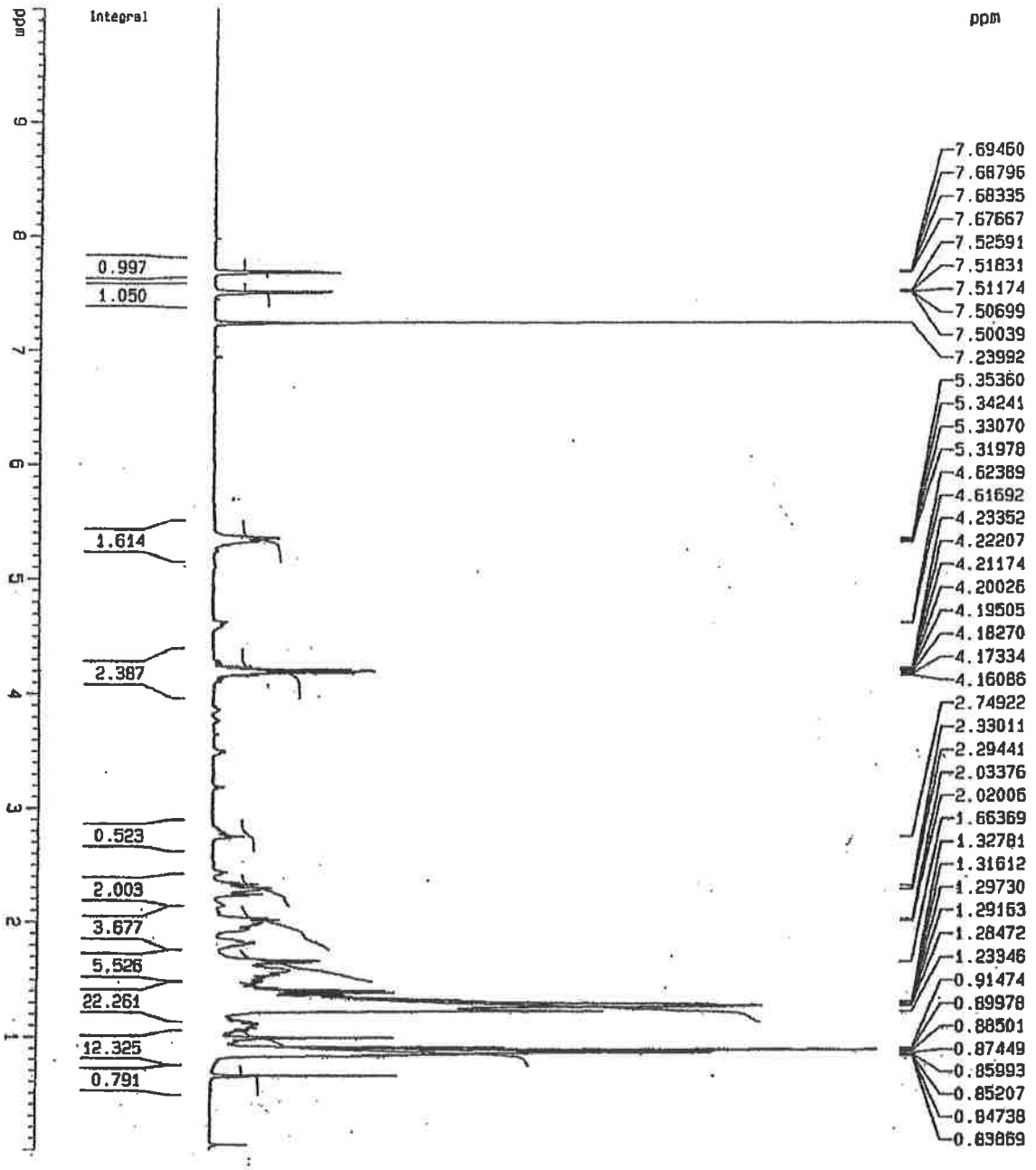

Integral
ppm
0.997
1.050
1.614
2.387
0.523
2.003
3.677
5.526
22.261
12.325
0.791
7.69460
7.68796
7.68335
7.67667
7.52591
7.51831
7.51174
7.50699
7.50039
7.23992
5.35360
5.34241
5.33070
5.31978
4.62389
4.61692
4.23352
4.22207
4.21174
4.20026
4.19505
4.18270
4.17334
4.16086
2.74922
2.33011
2.29441
2.03376
2.02006
1.66369
1.32781
1.31612
1.29730
1.29163
1.28472
1.23946
0.91474
0.89978
0.88501
0.87449
0.85993
0.85207
0.84738
0.83869

Figure 13

(a)

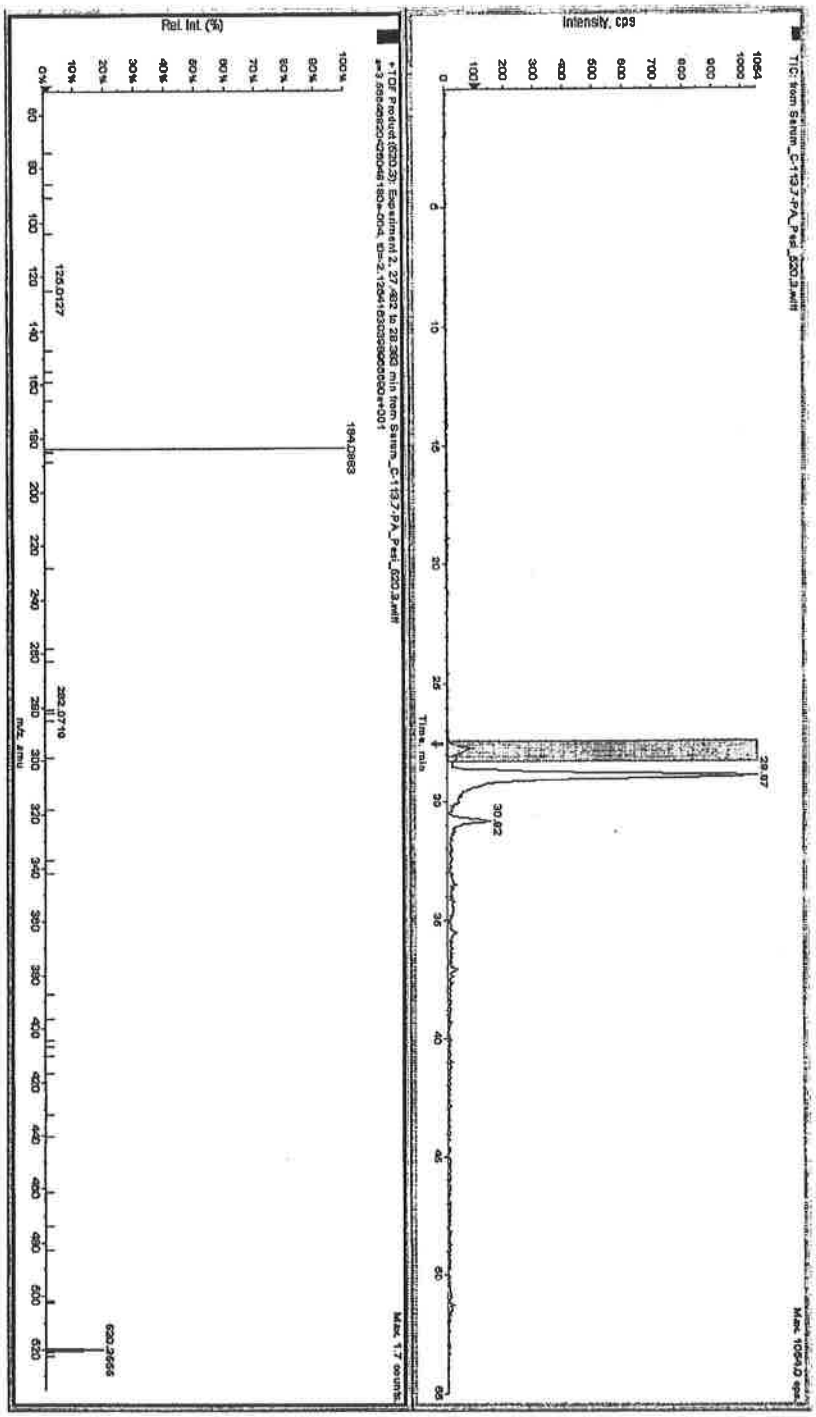

Rel. Int. (%)
Intensity, cps
Time, min
m/z, amu
125.0127
194.0883
282.0710
630.2656
29.87
30.62

Figure 14

(b)

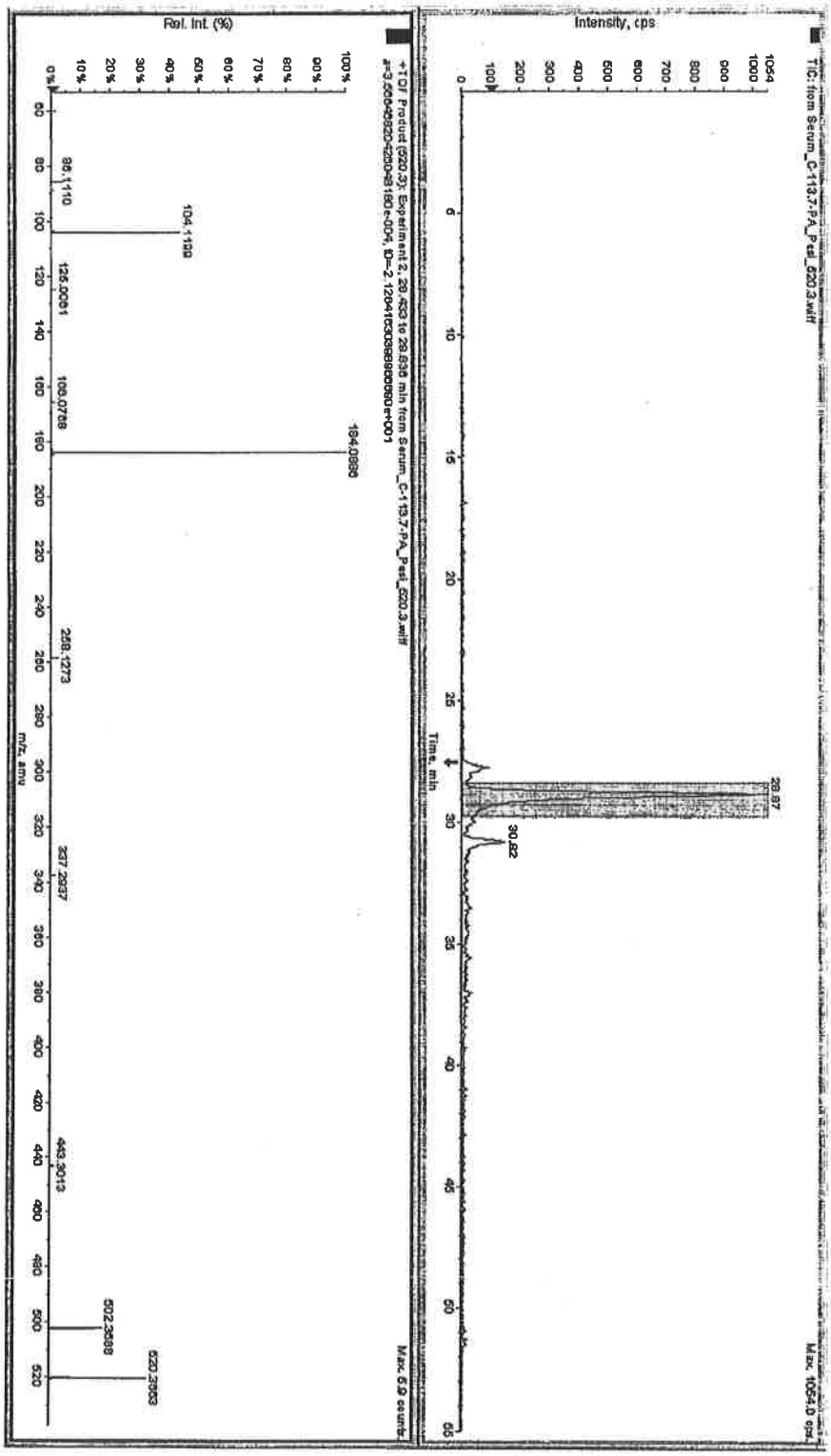


Figure 14 (cont.)

(a)

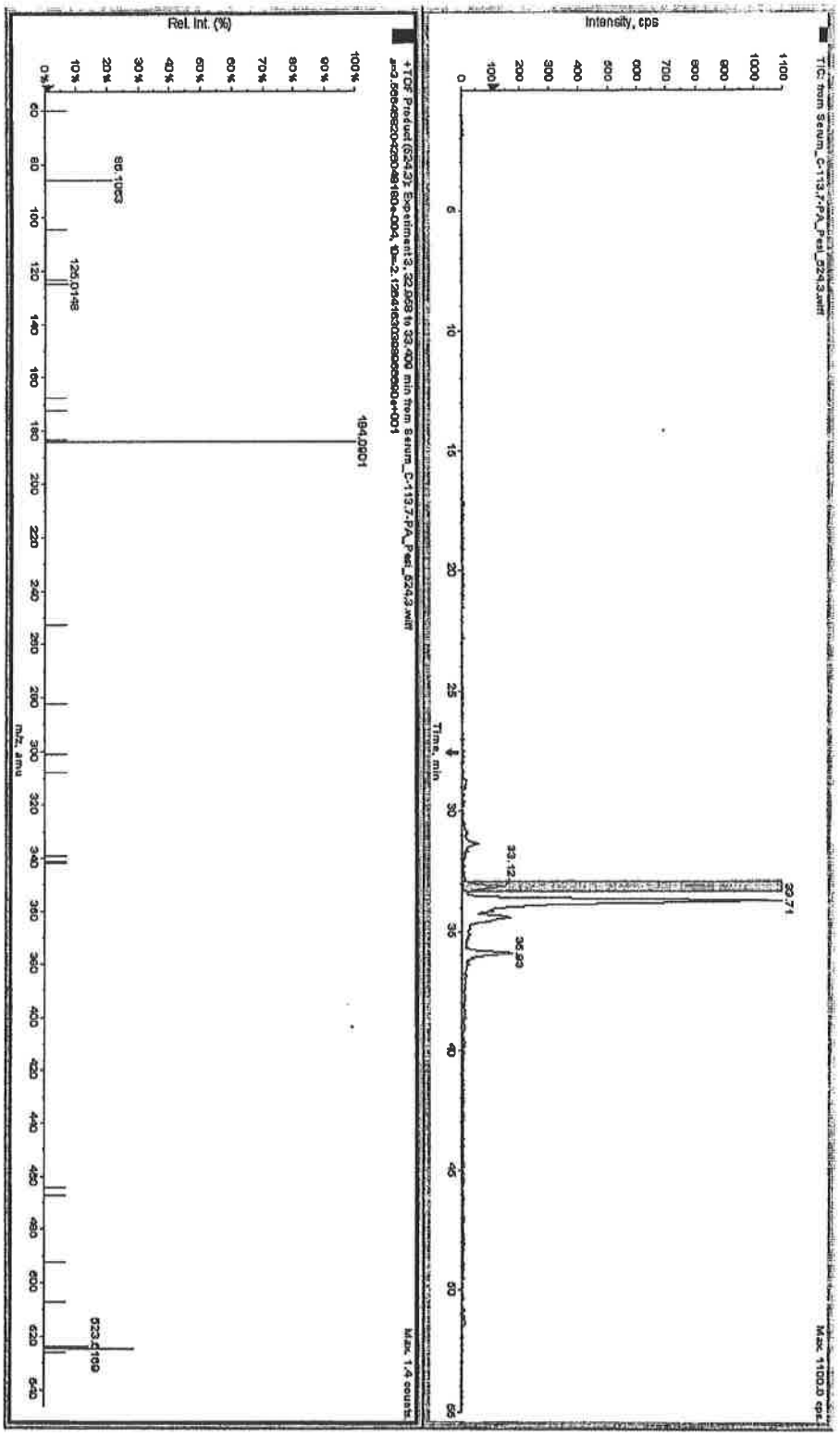

Intensity, cps
TIC: from Serum_C-113.7-PA_Pest_5243.wiff
Max. 1100.0 cps.
Time, min
23.12
29.71
35.89
Rel. Int. (%)
+TOF Product (5243): Experiment 3, 32.958 to 33.400 min from Serum_C-113.7-PA_Pest_5243.wiff
Max. 1.4 counts.
m/z, amu
194.0901
85.1063
120.0148
523.4169

Figure 15

(b)

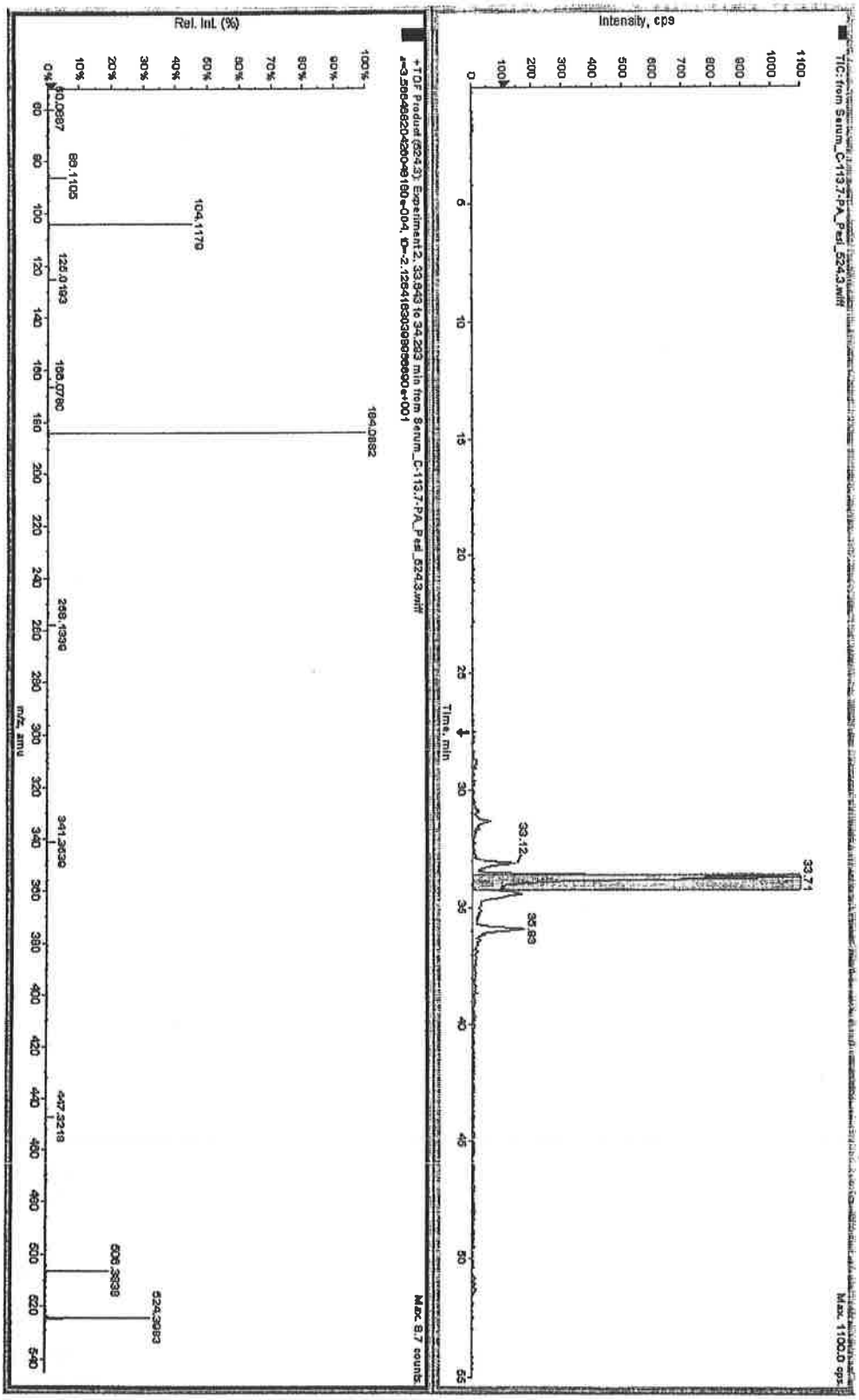


Figure 15 (cont.)

(a)

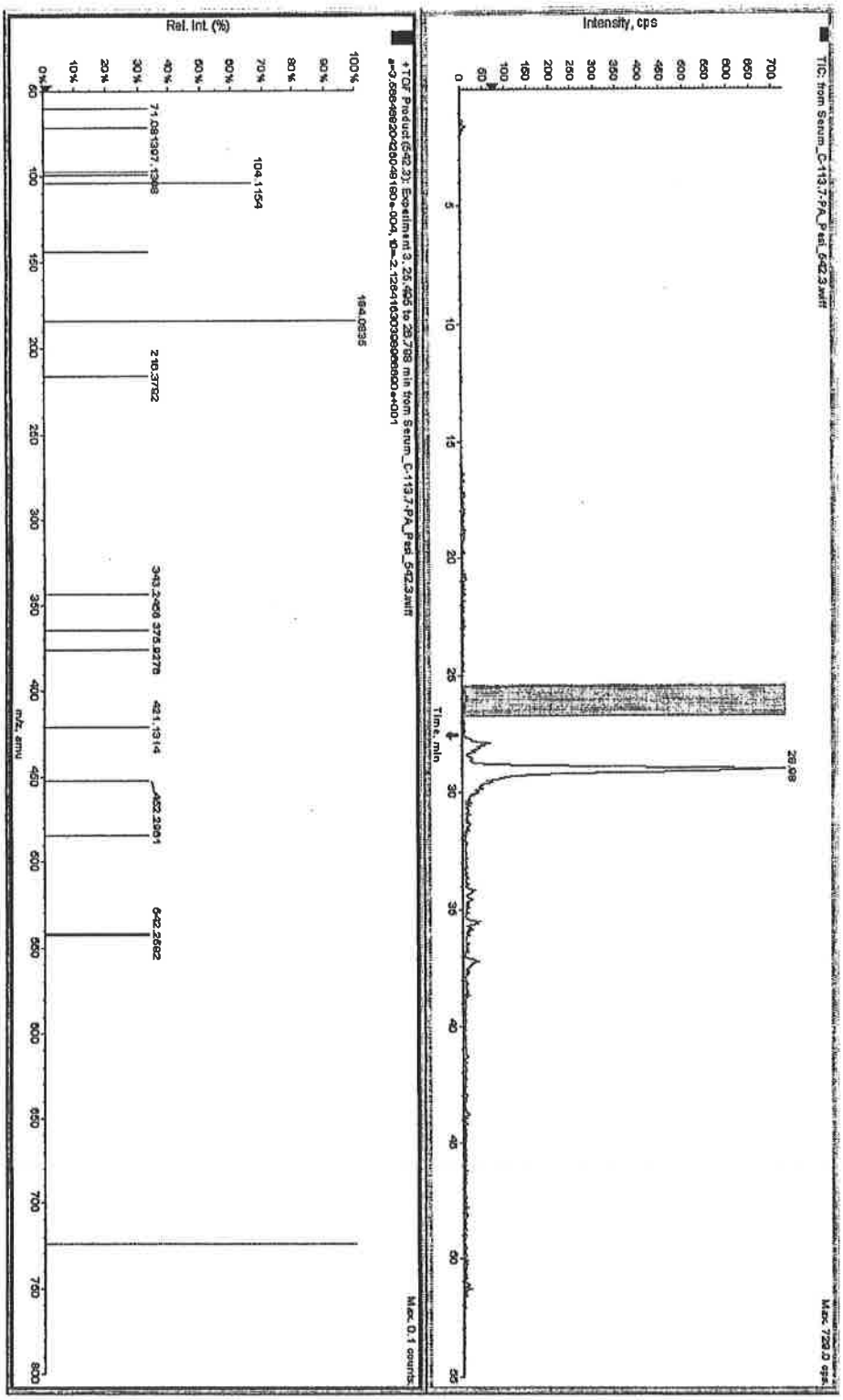

TIC: from Serum_C-113.7-PA_Pest_542.3.wiff
Intensity, cps
Time, min
Max. 723.0 cps.
29.98
+TOF Product (542.3): Experiment 3, 25.426 to 29.798 min from Serum_C-113.7-PA_Pest_542.3.wiff
Rel. Int. (%)
m/z, amu
Max. 0.1 counts.
71.081397
104.1154
164.0935
216.3702
343.2450
375.9278
421.1314
452.2901
642.2662

Figure 16

(b)

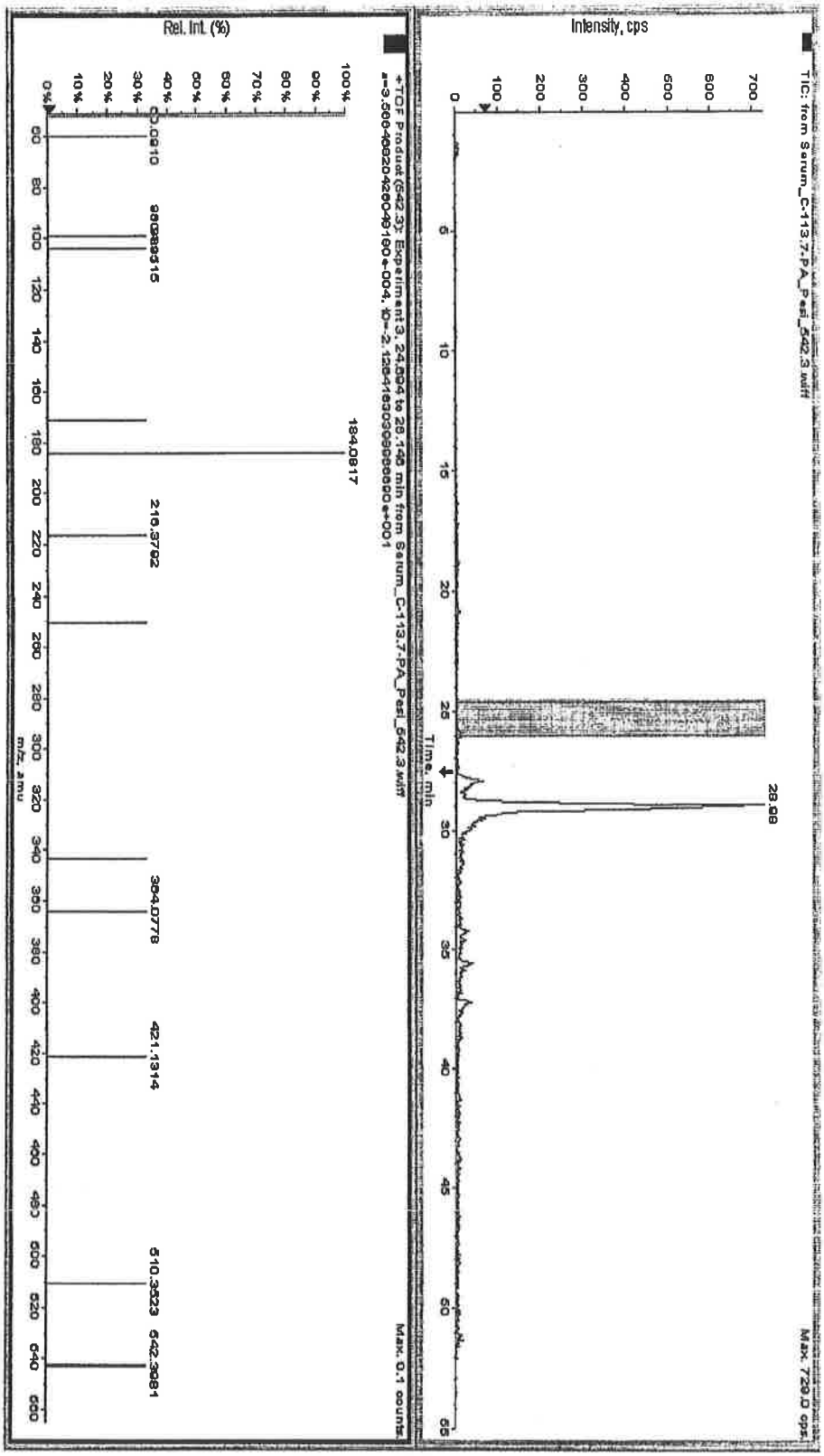


Figure 16 (cont.)

(c)

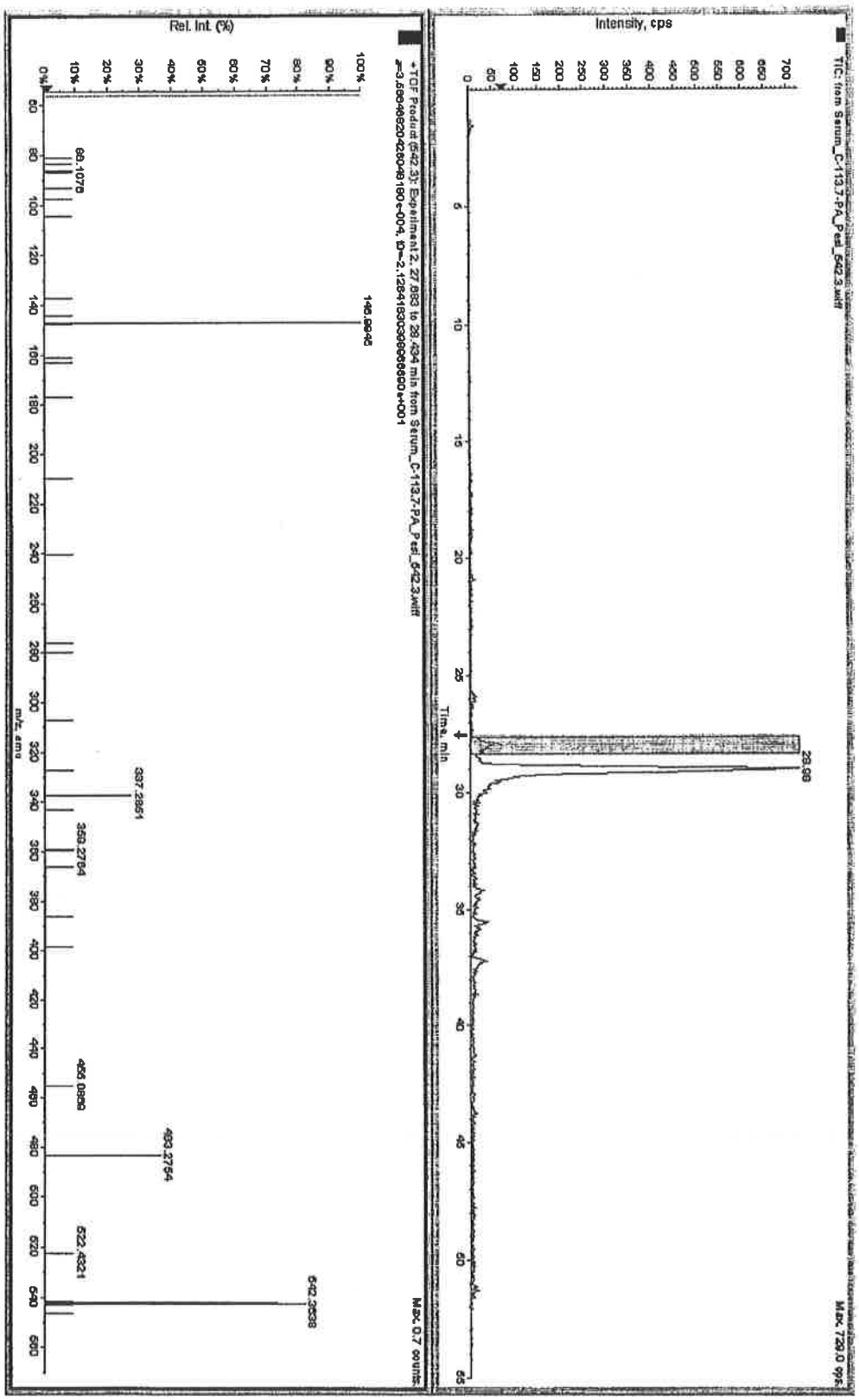


Figure 16 (cont.)

(d)

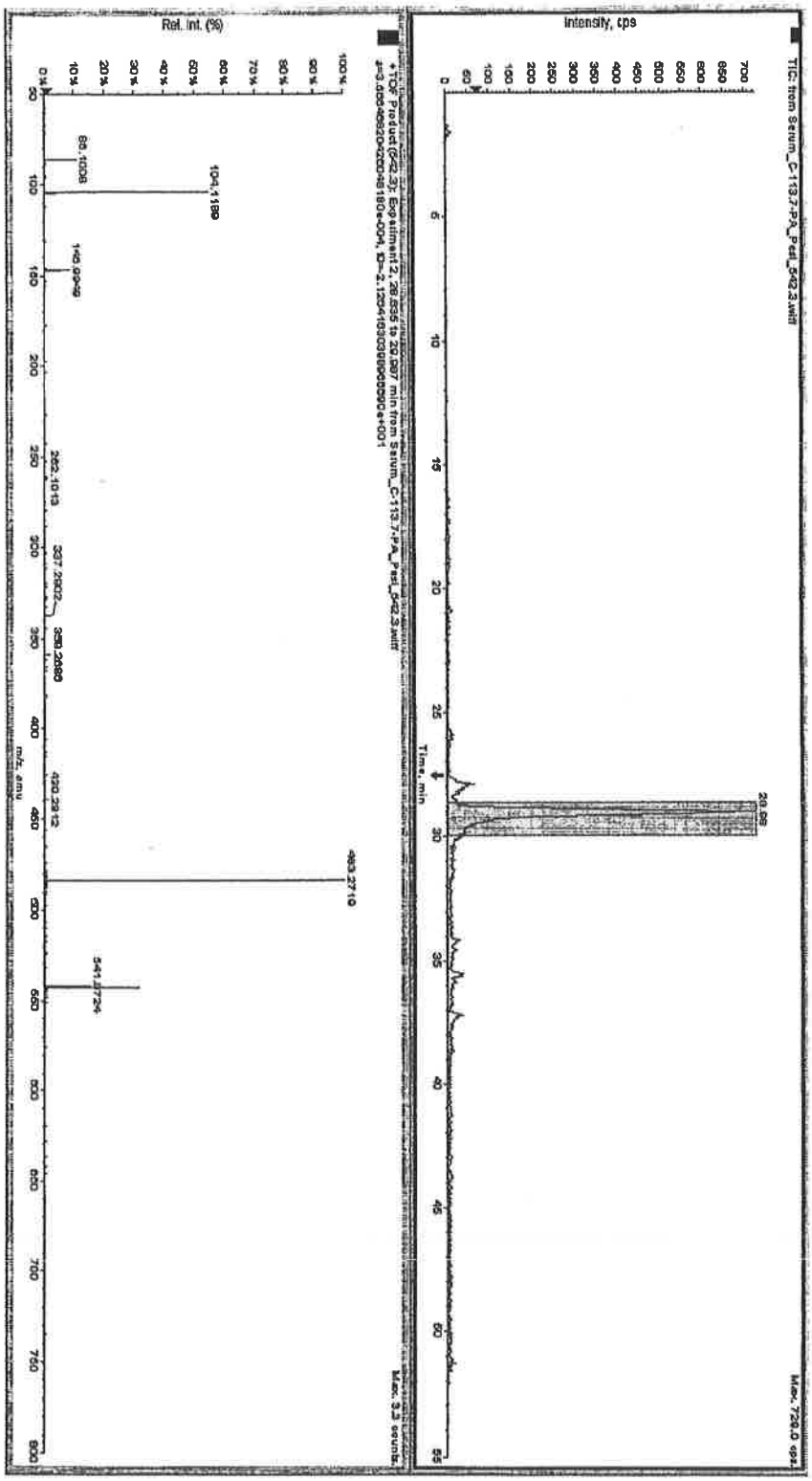


Figure 16 (cont.)

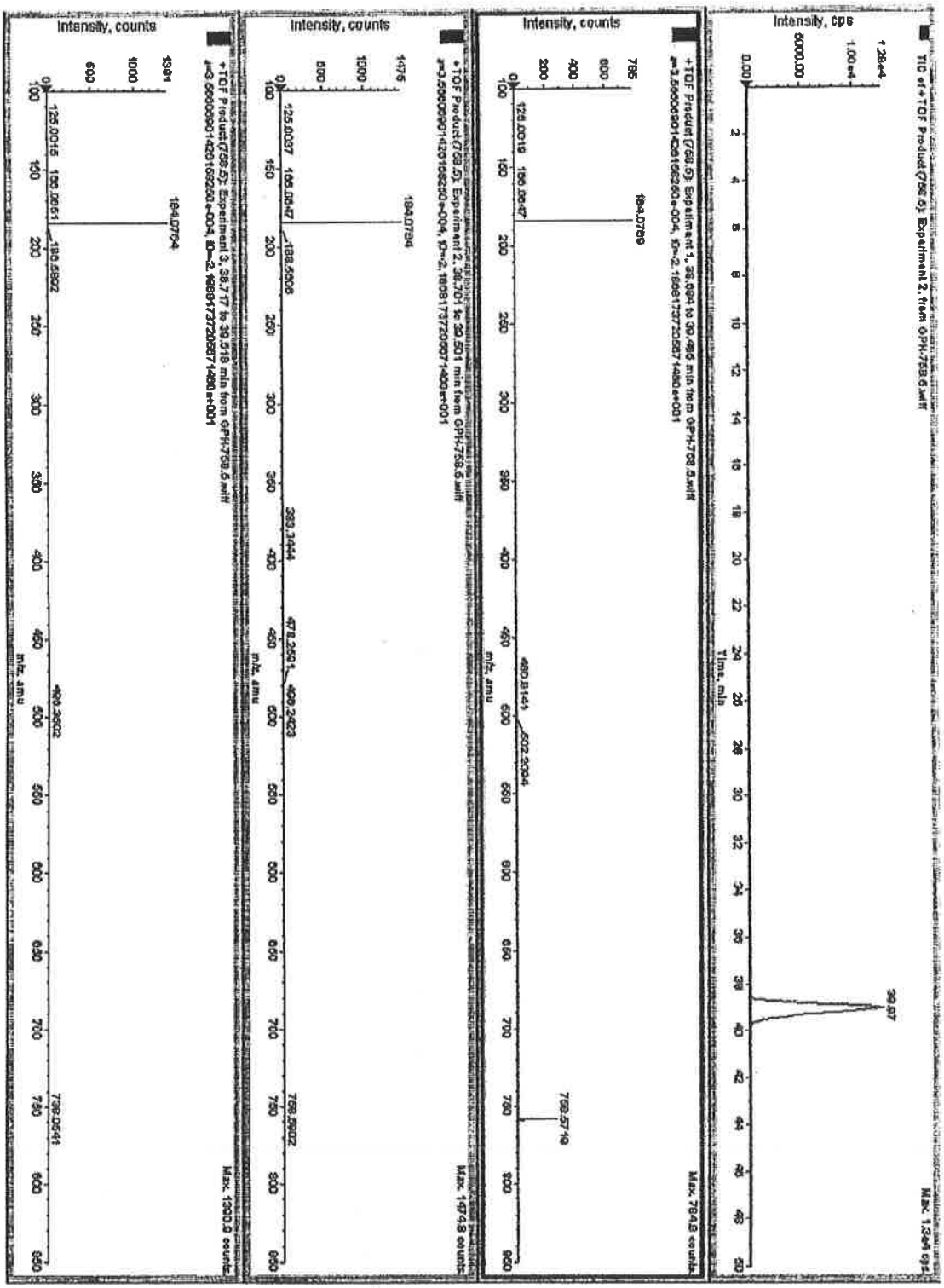

TIC of +TOF Product(758.5): Experiment 2, from GPH-758.5.wiff
Intensity, cps
Time, min
39.87
Max. 1.3e+5 cps.
+TOF Product(758.5): Experiment 1, 38.094 to 39.485 min from GPH-758.5.wiff
Intensity, counts
184.0789
125.0019
166.0647
480.8141
502.2094
792.5749
Max. 7648 counts.
+TOF Product(758.5): Experiment 2, 38.701 to 39.501 min from GPH-758.5.wiff
Intensity, counts
184.0784
125.0037
166.0647
383.3444
478.2491
409.2423
758.5902
Max. 1474.8 counts.
+TOF Product(758.5): Experiment 3, 38.717 to 39.518 min from GPH-758.5.wiff
Intensity, counts
184.0784
125.0015
166.0651
189.5802
409.3602
738.0641
Max. 1380.0 counts.
m/z, amu

Figure 17

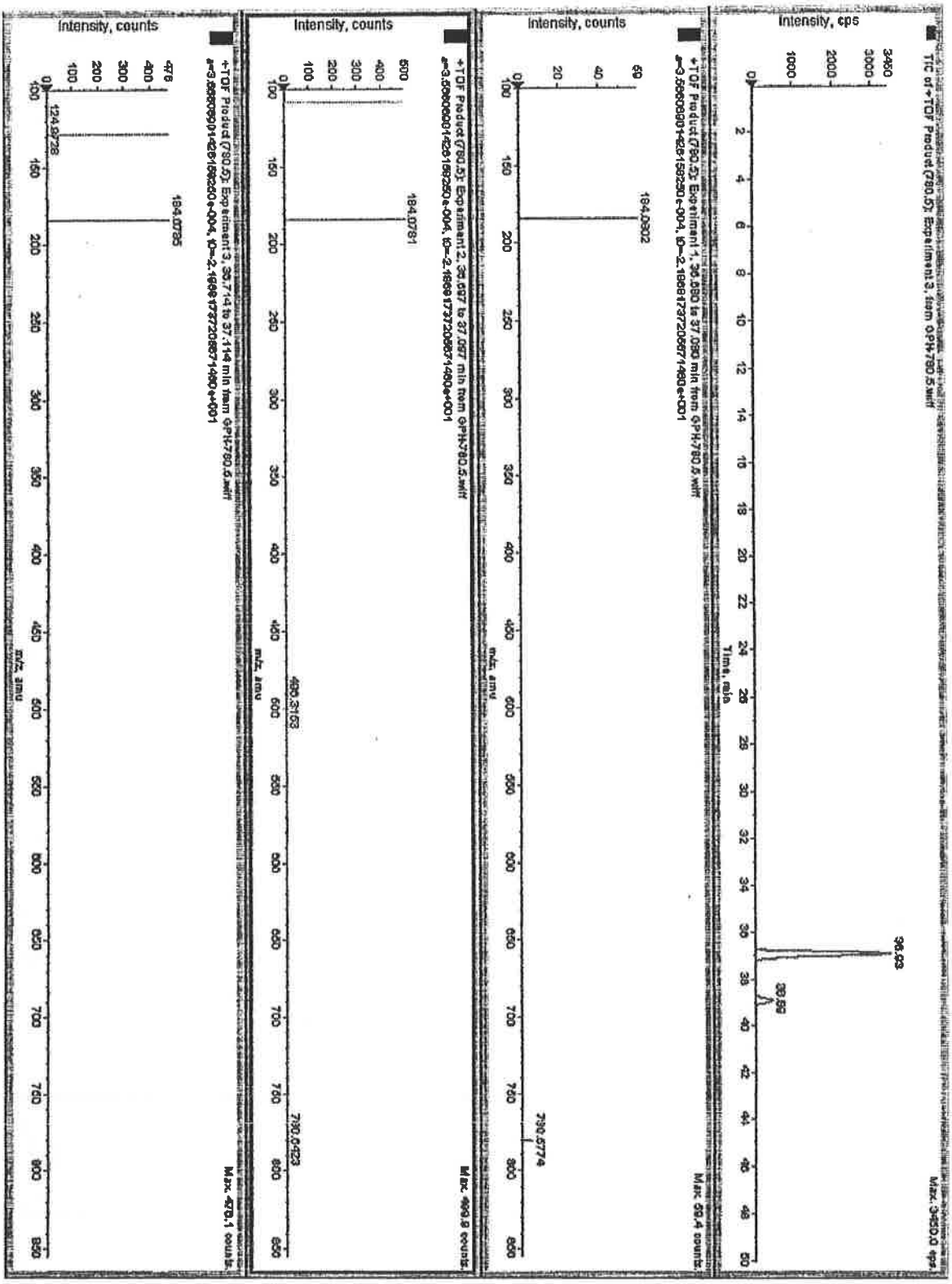

TIC of +TOF Product (780.5) Experiment 3, from GPH-780.5.wiff
Intensity, cps
Time, min
36.93
39.59
Max: 3450.0 cps.
+TOF Product (780.5): Experiment 1, 36.680 to 37.090 min from GPH-780.5.wiff
Intensity, counts
184.0802
790.5774
Max: 69.4 counts.
+TOF Product (780.5): Experiment 2, 36.597 to 37.007 min from GPH-780.5.wiff
Intensity, counts
184.0781
490.3163
790.5423
Max: 499.9 counts.
+TOF Product (780.5): Experiment 3, 36.714 to 37.114 min from GPH-780.5.wiff
Intensity, counts
476
184.0785
124.0728
Max: 478.1 counts.
m/z, amu

Figure 18

(a)

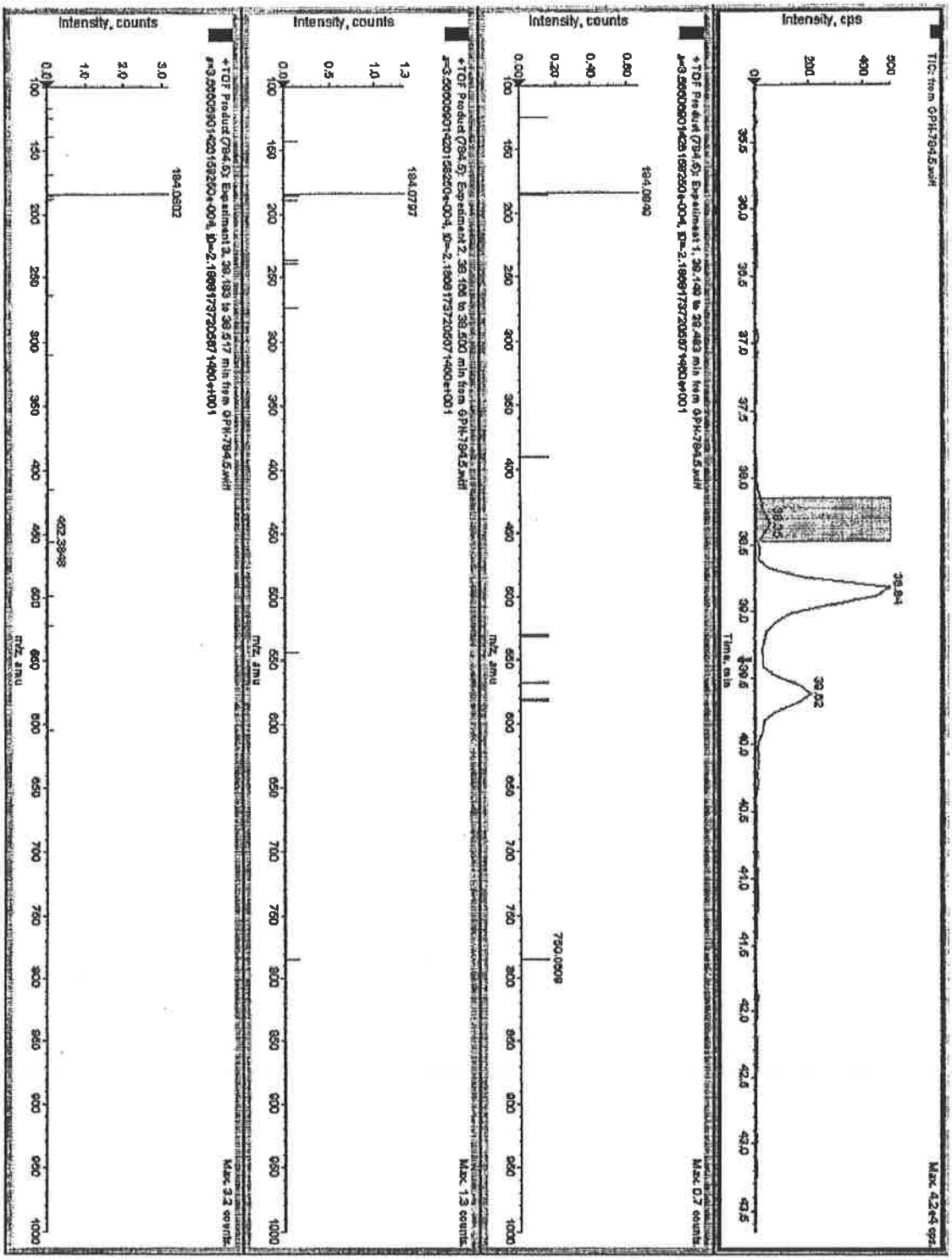

Intensity, cps
Time, min
Intensity, counts
m/z, amu
184.0840
750.0509
184.0787
184.0802
402.2948

Figure 19

(b)

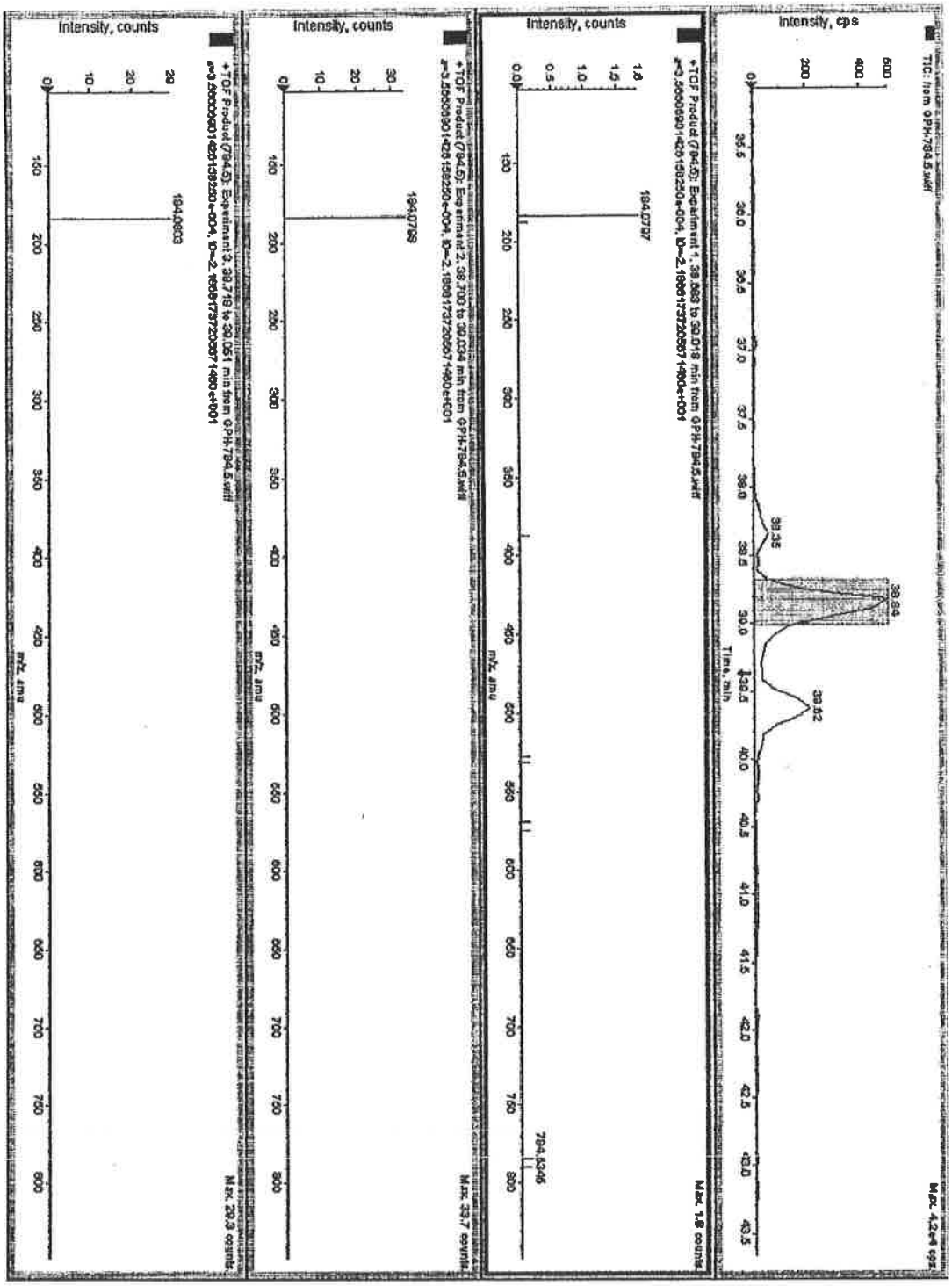


Figure 19 (Cont.)

(c)

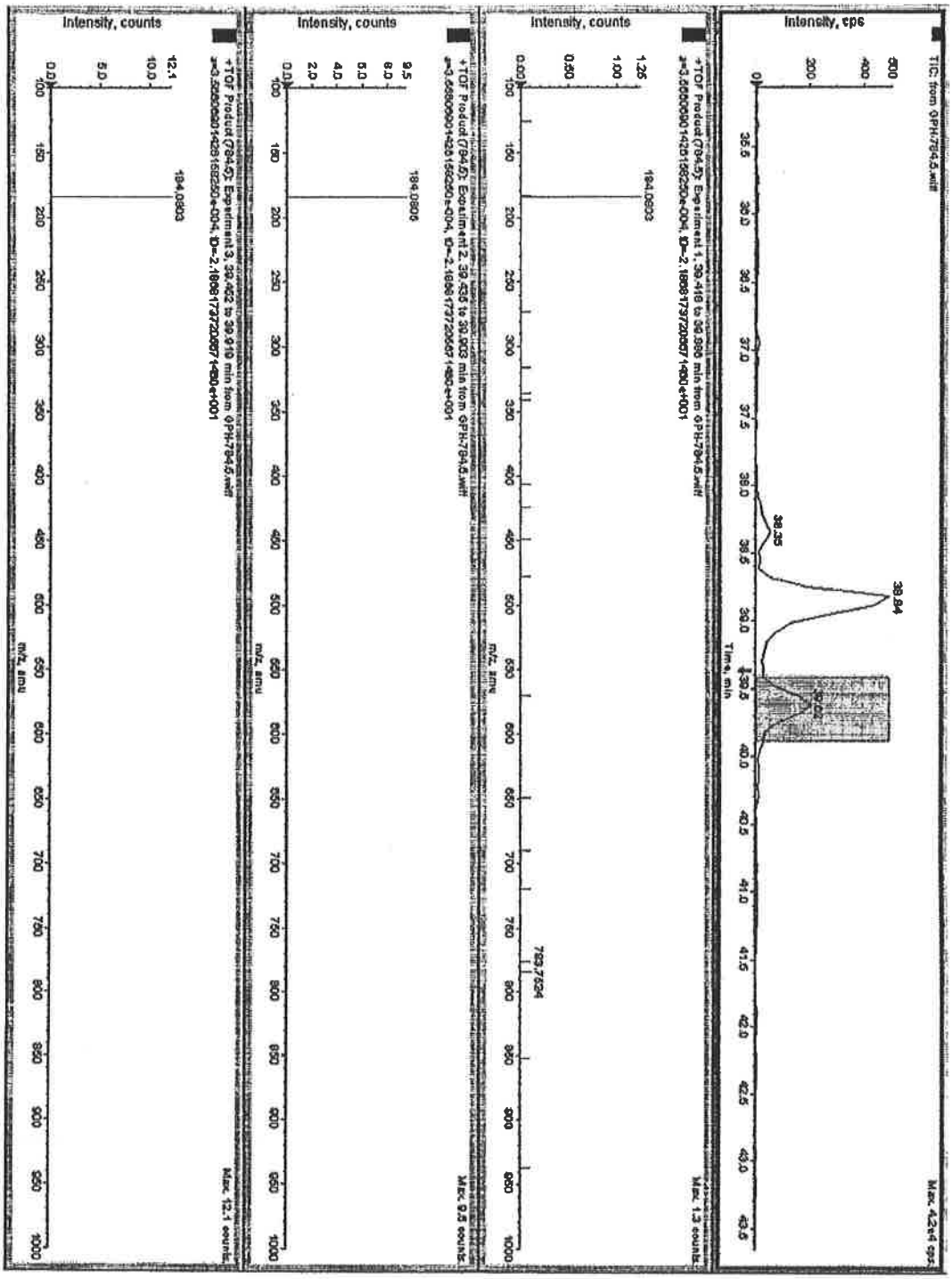


Figure 19 (Cont.)

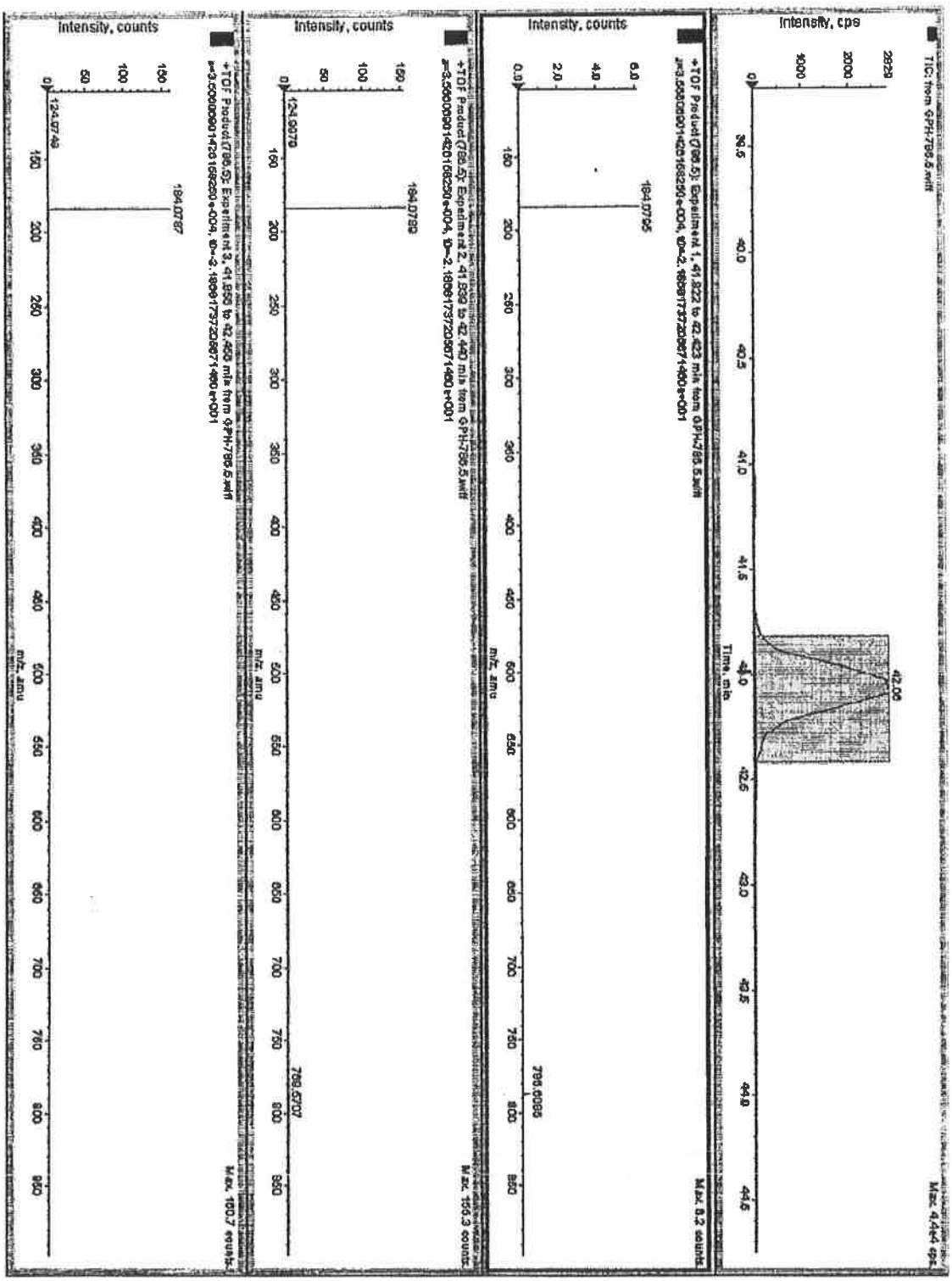

TIC from QPH-795.5.wiff
Max. 4.4e4 cps.
Intensity, cps
Time, min
42.06
+TOF Product(795.5): Experiment 1, 41.822 to 42.423 min from QPH-795.5.wiff
Max. 8.2 counts
Intensity, counts
184.0795
795.5095
+TOF Product(795.5): Experiment 2, 41.838 to 42.440 min from QPH-795.5.wiff
Max. 155.3 counts
184.0789
795.5707
+TOF Product(795.5): Experiment 3, 41.856 to 42.458 min from QPH-795.5.wiff
Max. 100.7 counts
124.0749
184.0787
m/z, amu

Figure 20

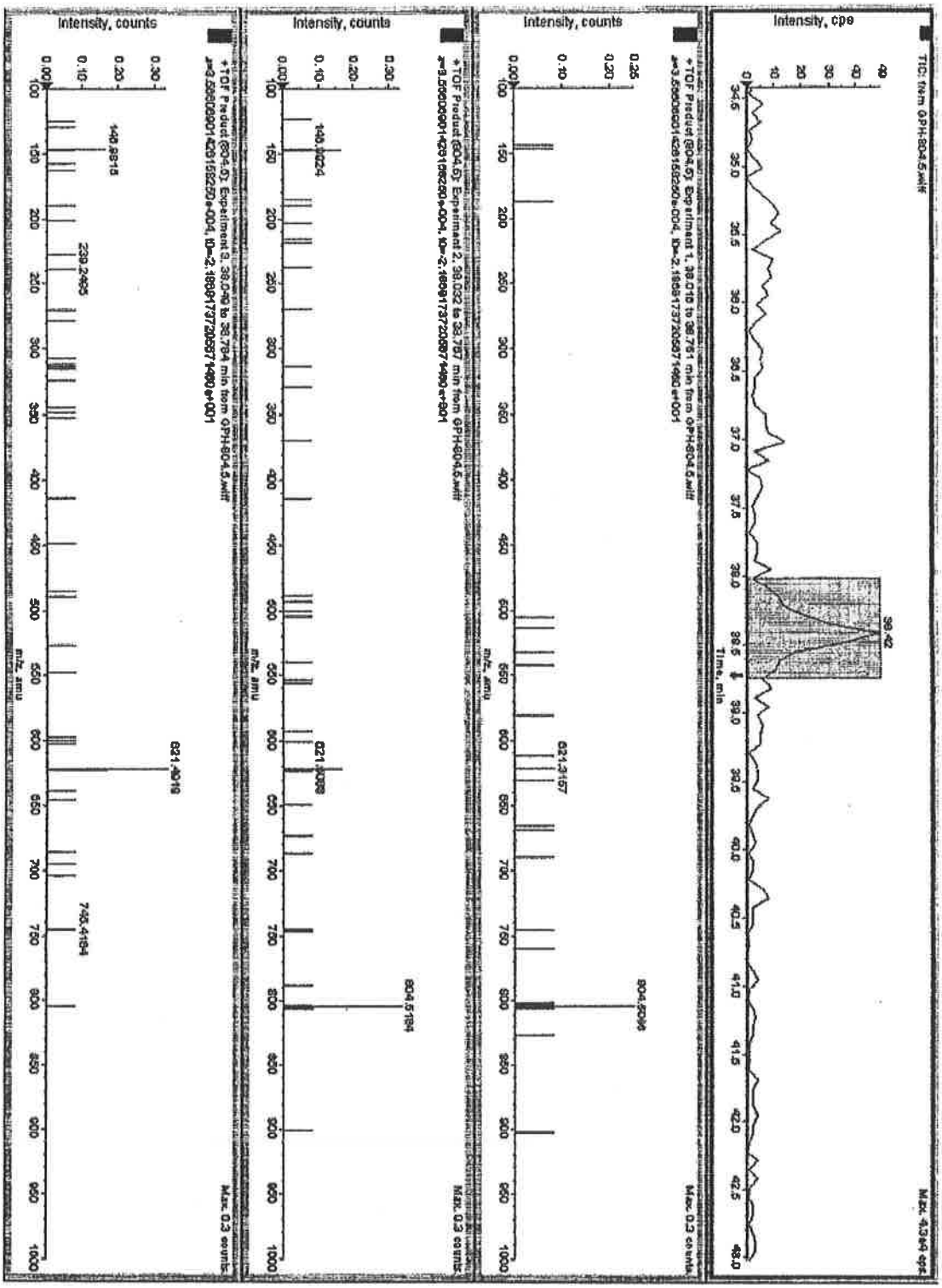

Intensity, cps
Time, min
Intensity, counts
m/z, amu
804.5094
621.3157
804.5184
621.3008
745.4194
621.4016
239.2405
149.0224
148.9815

Figure 21

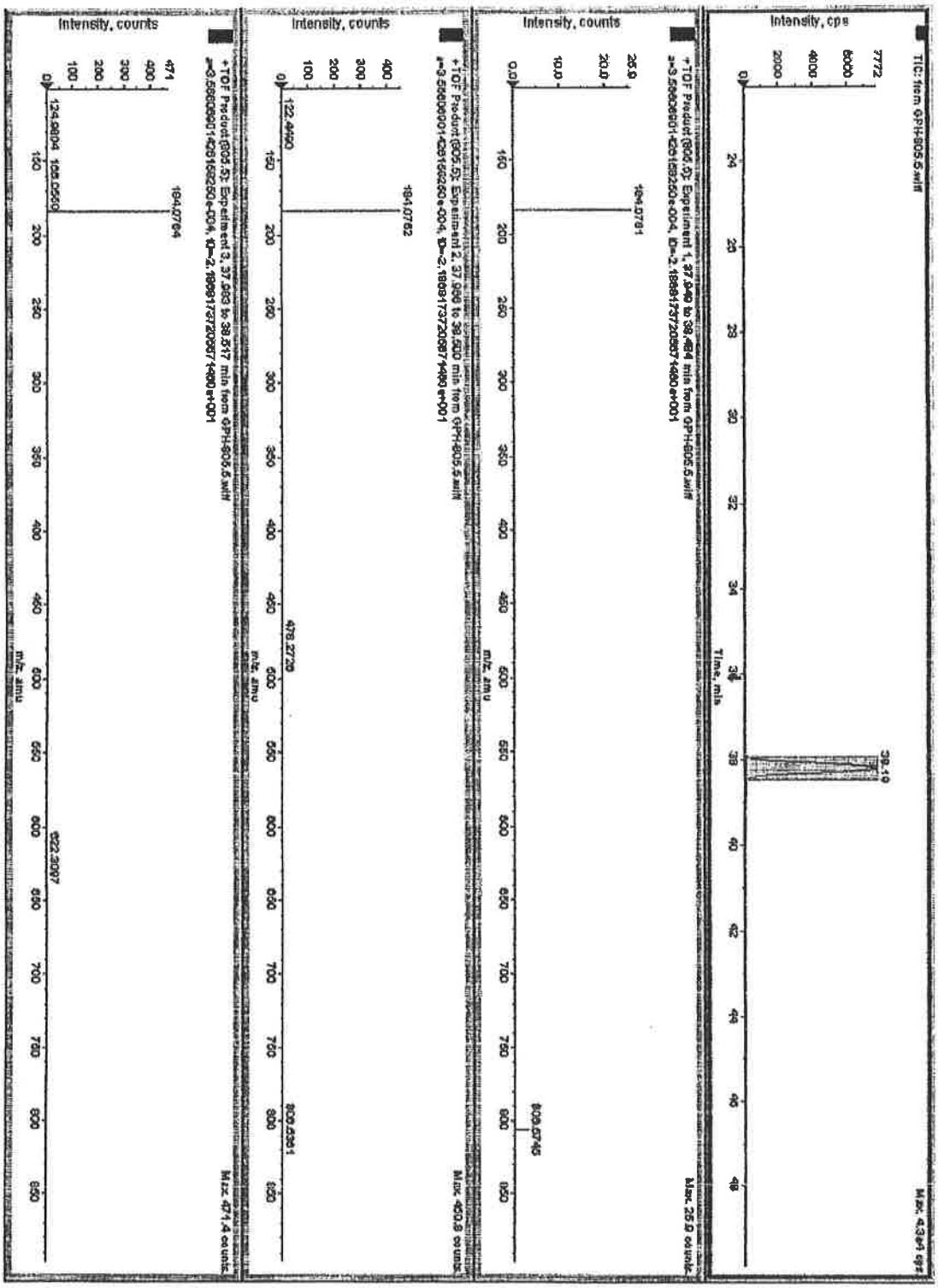

TIC: from QPH-605.5.wiff
Intensity, cps
Time, min
39.19
Intensity, counts
m/z, amu
194.0781
909.5745
194.0762
479.2729
909.5361
194.0764
922.3097
124.9804
155.0559

Figure 22

(a)

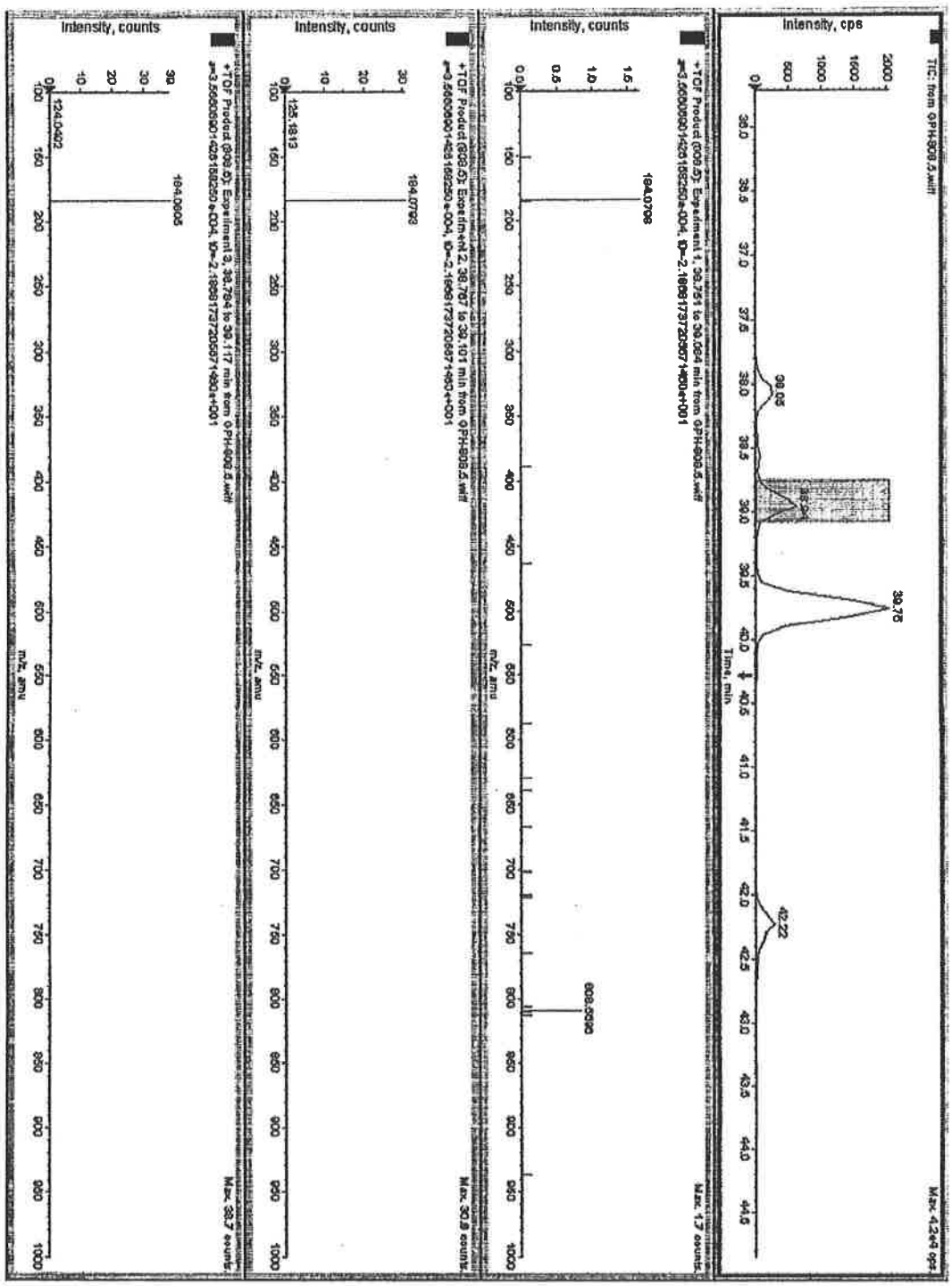

TIC: from GPH-908.5.wiff
Max: 4.2e+9 cps
Intensity, cps
Time, min
38.05
38.76
42.22
+TOF Product (908.5): Experiment 1, 38.751 to 39.064 min from GPH-908.5.wiff
Max: 1.7 counts
Intensity, counts
184.0708
908.5936
+TOF Product (908.5): Experiment 2, 38.787 to 39.101 min from GPH-908.5.wiff
Max: 30.8 counts
125.1813
184.0703
+TOF Product (908.5): Experiment 3, 38.784 to 39.117 min from GPH-908.5.wiff
Max: 38.7 counts
124.0402
184.0605
m/z, amu

Figure 23

(b)

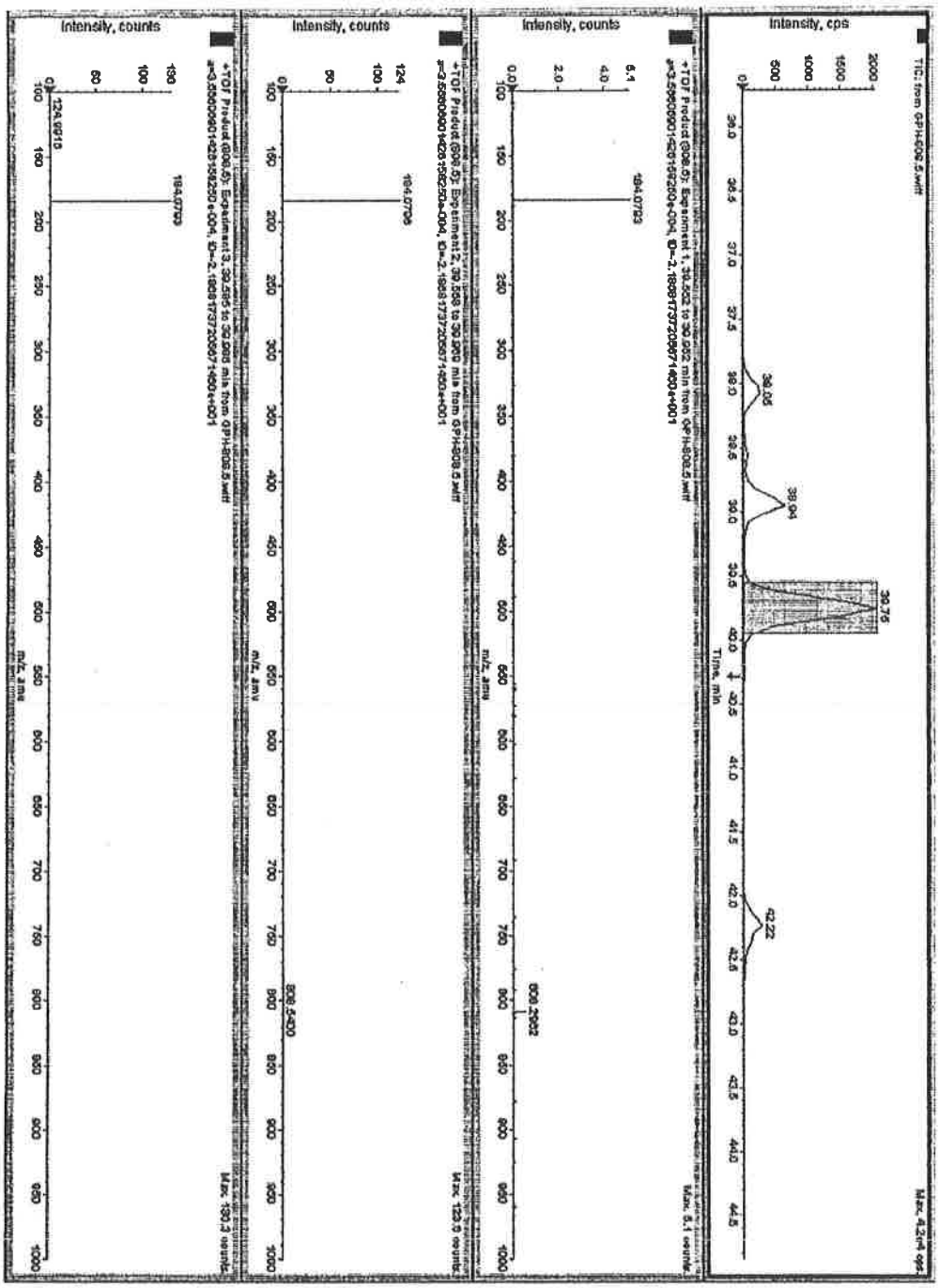


Figure 23 (Cont.)

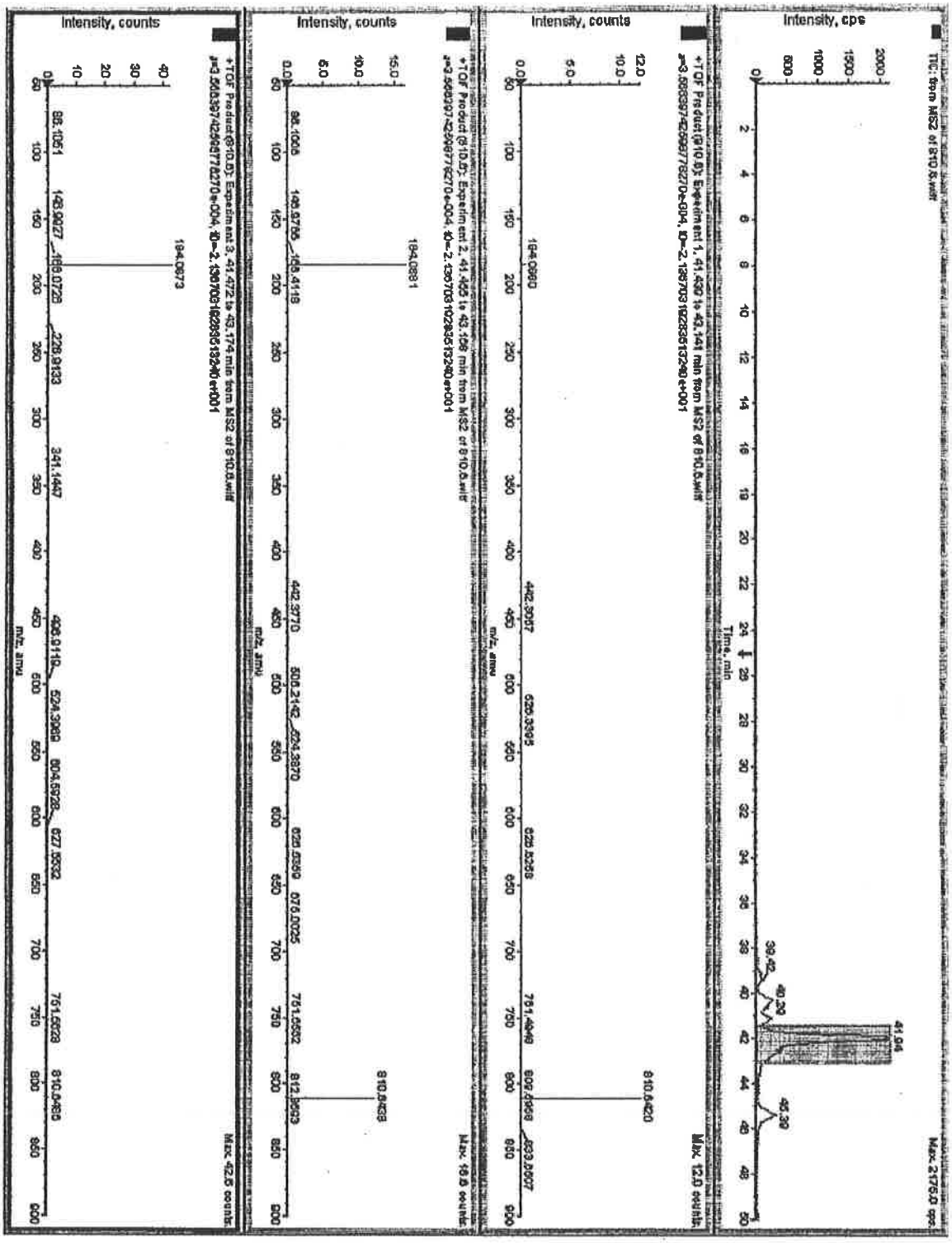

TIC: from MS2 of 810.5.wiff
Max. 2175.0 cps.
Intensity, cps
Time, min
41.94
40.20
39.42
45.39
+TOF Product (810.5): Experiment 1, 41.430 to 43.141 min from MS2 of 810.5.wiff
Max. 12.0 counts.
Intensity, counts
810.5420
194.0860
+TOF Product (810.5): Experiment 2, 41.485 to 43.198 min from MS2 of 810.5.wiff
Max. 18.0 counts.
Intensity, counts
810.5439
194.0881
+TOF Product (810.5): Experiment 3, 41.472 to 43.174 min from MS2 of 810.5.wiff
Max. 42.5 counts.
Intensity, counts
194.0873
m/z, amu

Figure 24

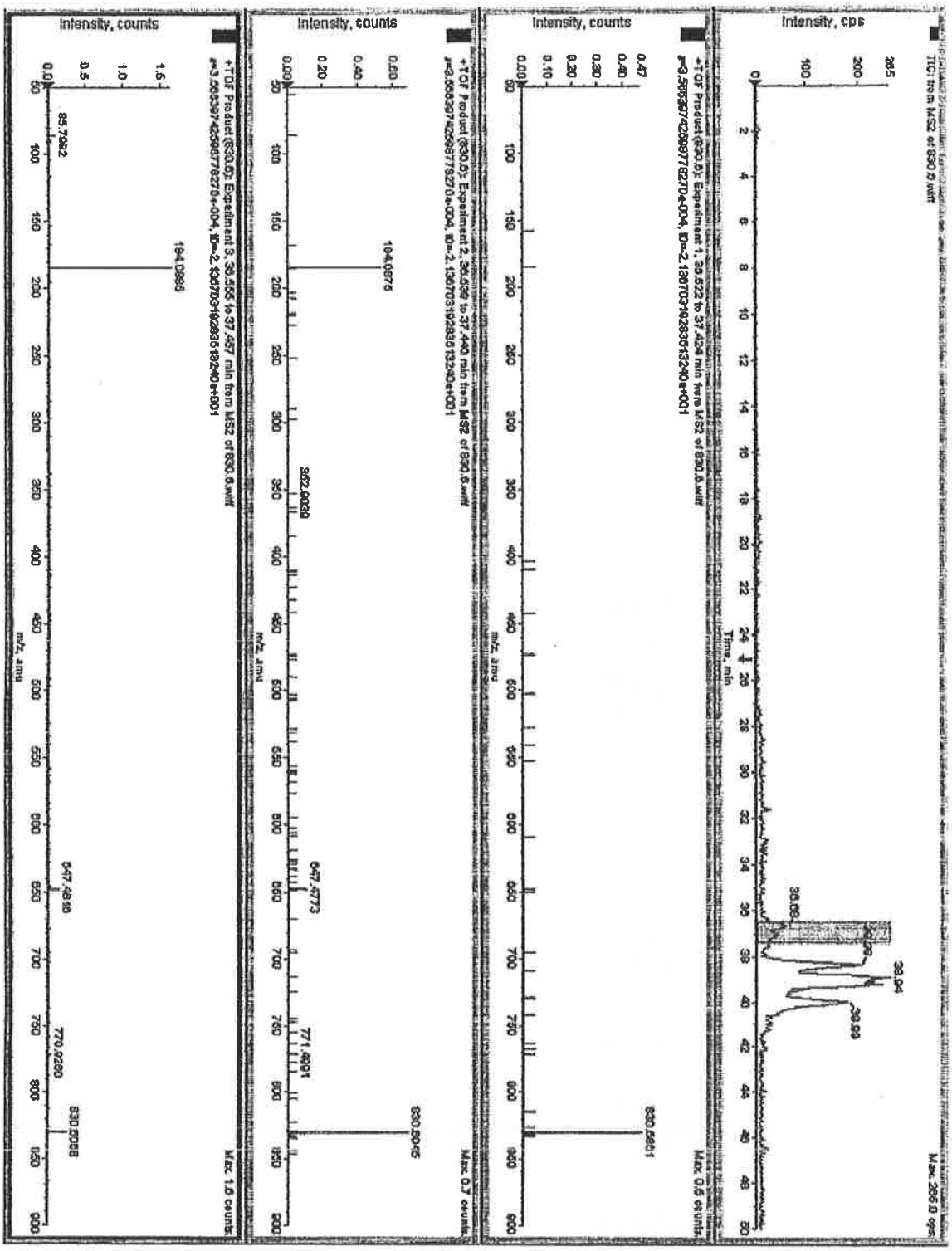

Intensity, cps
Time, min
Intensity, counts
m/z, amu
194.0865
85.7982
647.4816
770.9280
830.5068
194.0875
352.9039
647.4773
771.4991
830.5045
830.5051

Figure 25

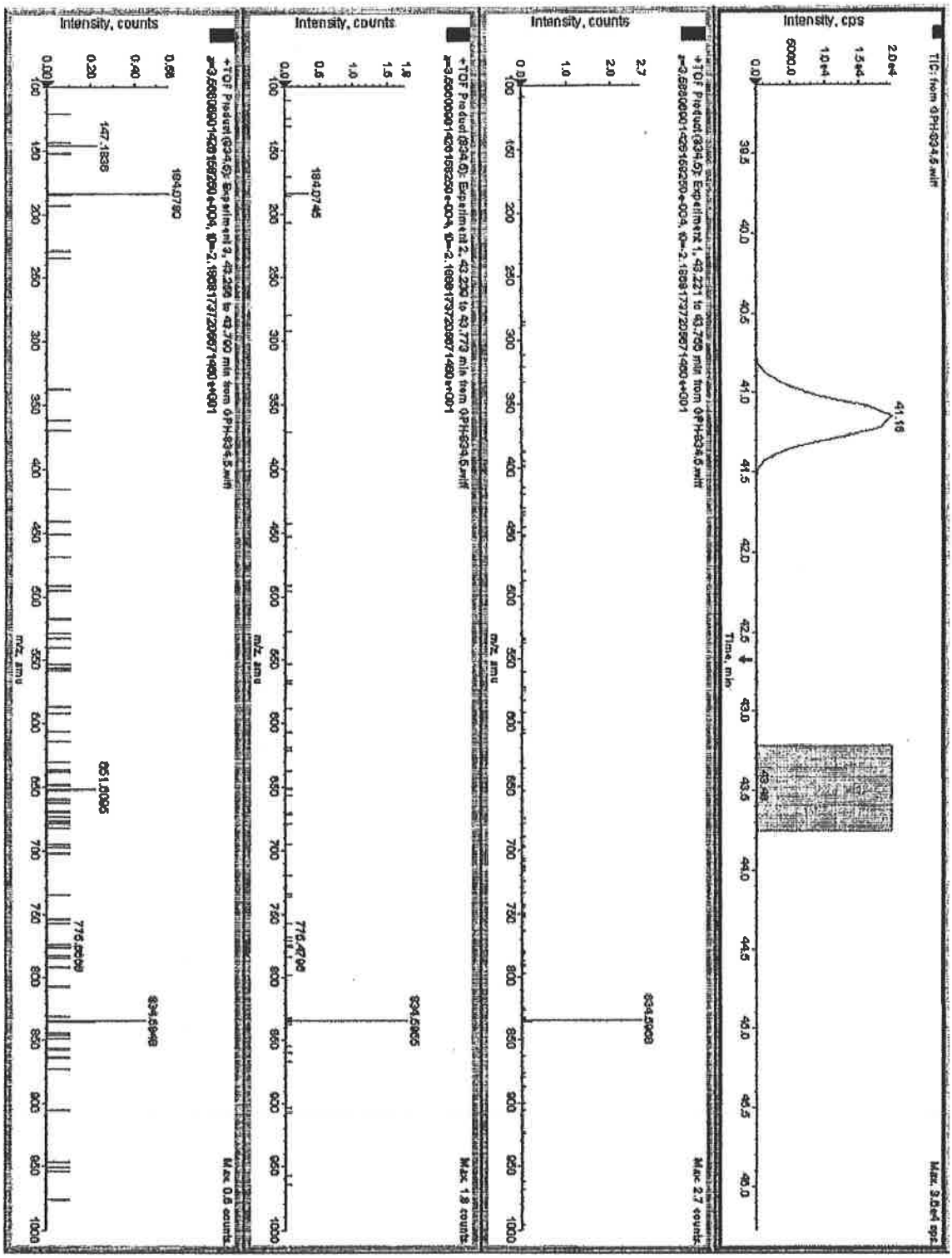

TIC: from 6PH-934-5.wiff
Intensity, cps
Max. 3.5e4 cps.
41.16
Time, min
+TDF Product(934.6): Experiment 1, 40.221 to 43.769 min from 6PH-934-5.wiff
Intensity, counts
Max. 2.7 counts.
934.5968
+TDF Product(934.6): Experiment 2, 40.230 to 43.779 min from 6PH-934-5.wiff
Max. 1.8 counts.
934.5965
+TDF Product(934.6): Experiment 3, 40.265 to 43.760 min from 6PH-934-5.wiff
Max. 0.6 counts.
934.5968
m/z, amu

Figure 26

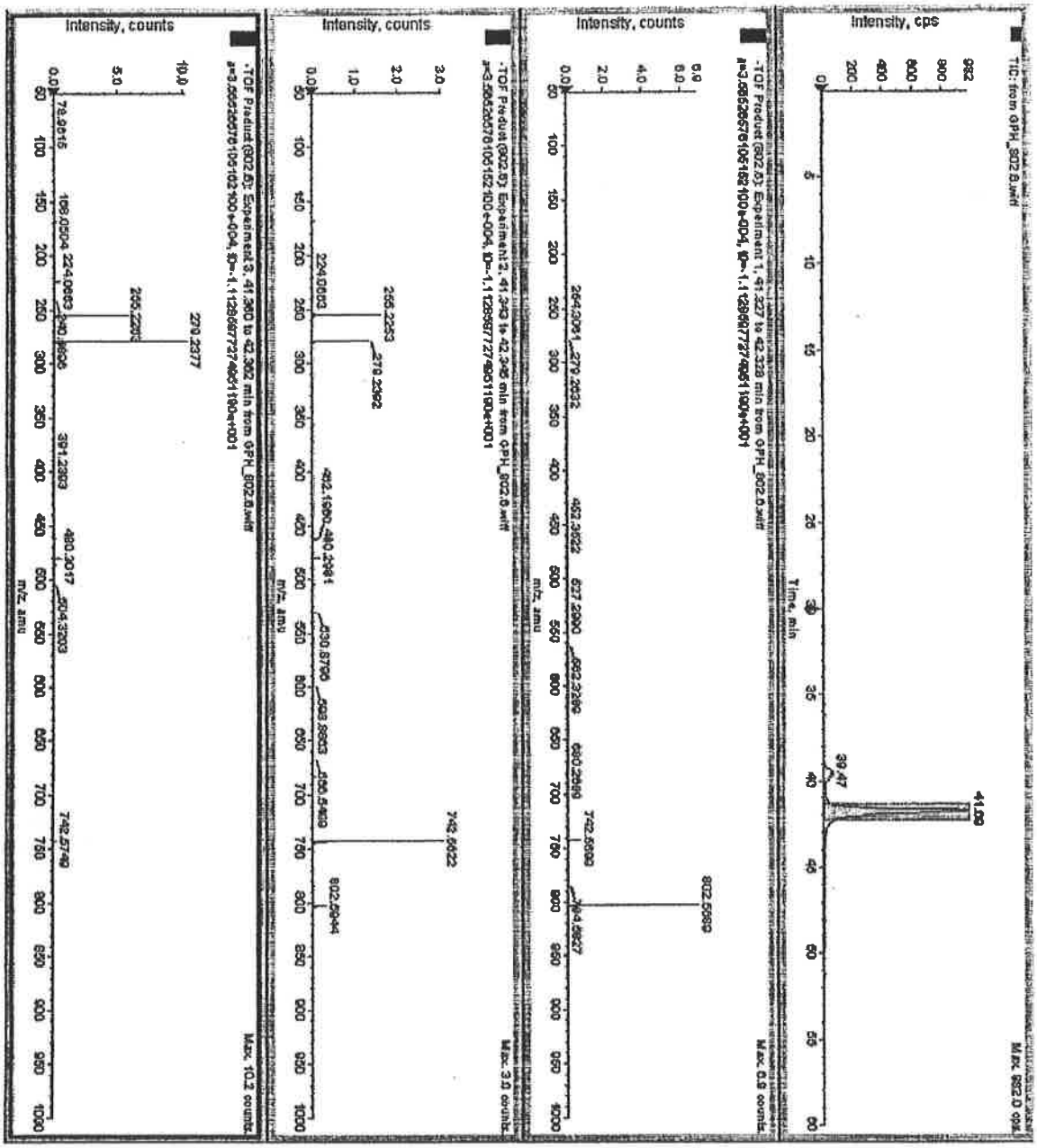

TIC: from GPH_802.0.wiff
Intensity, cps
Time, min
39.47
41.09
Max. 932.0 cps
-TOF Product (802.0): Experiment 1, 41.227 to 42.328 min from GPH_802.0.wiff
Intensity, counts
802.5689
744.5827
Max. 6.0 counts
-TOF Product (802.0): Experiment 2, 41.243 to 42.345 min from GPH_802.0.wiff
742.5822
Max. 3.0 counts
-TOF Product (802.0): Experiment 3, 41.360 to 42.362 min from GPH_802.0.wiff
279.2377
255.2253
224.0663
Max. 10.2 counts
m/z, amu

Figure 27

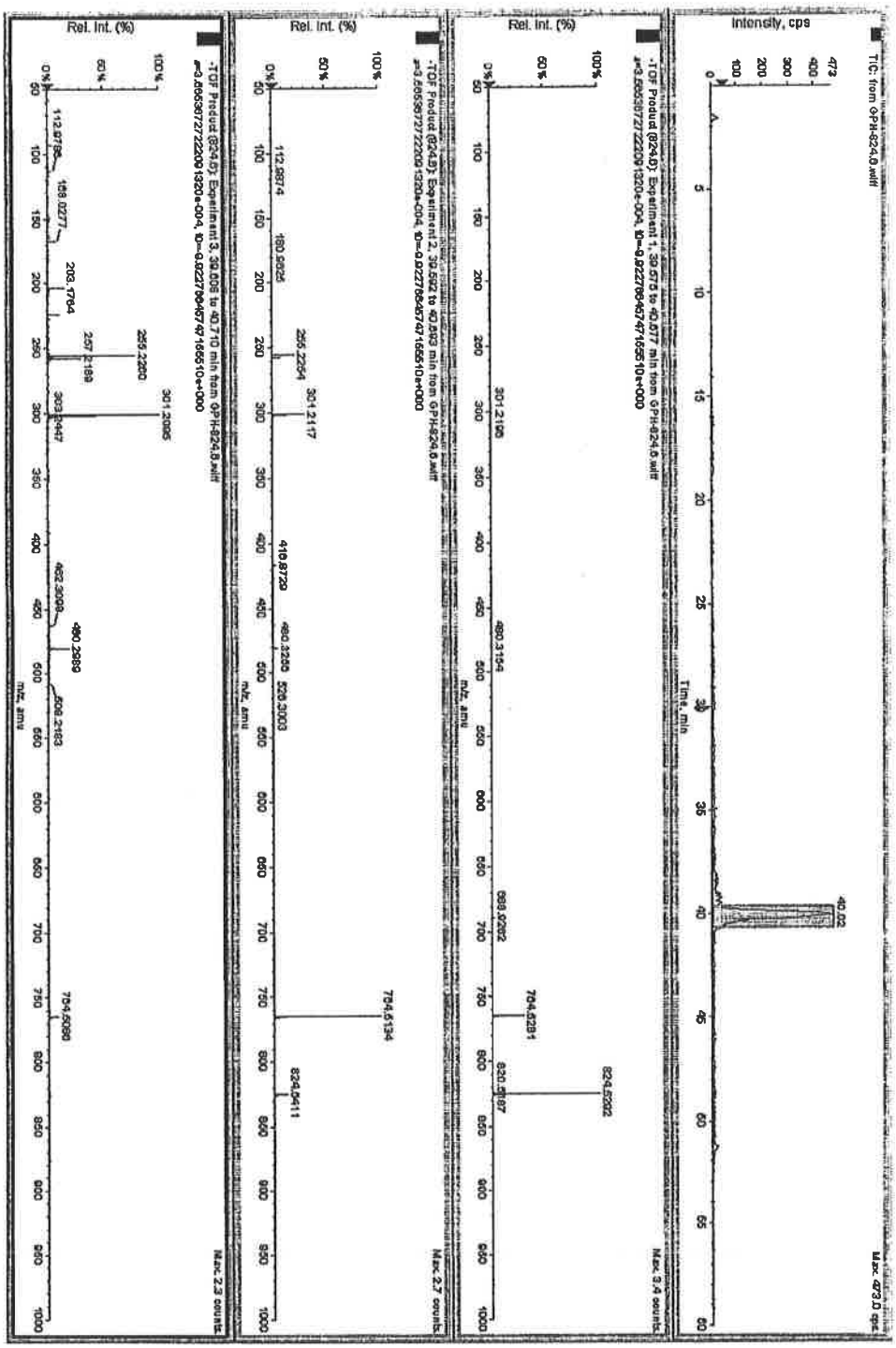

TIC: from 0PH-824.0.wiff
Intensity, cps
Time, min
Max. 473.0 cps.
-TOF Product (824.0): Experiment 1, 39.575 to 40.077 min from 0PH-824.0.wiff
Rel. Int. (%)
m/z, amu
Max. 3.4 counts.
-TOF Product (824.0): Experiment 2, 39.2921 to 40.093 min from 0PH-824.0.wiff
Max. 2.7 counts.
-TOF Product (824.0): Experiment 3, 39.606 to 40.710 min from 0PH-824.0.wiff
Max. 2.3 counts.

Figure 28

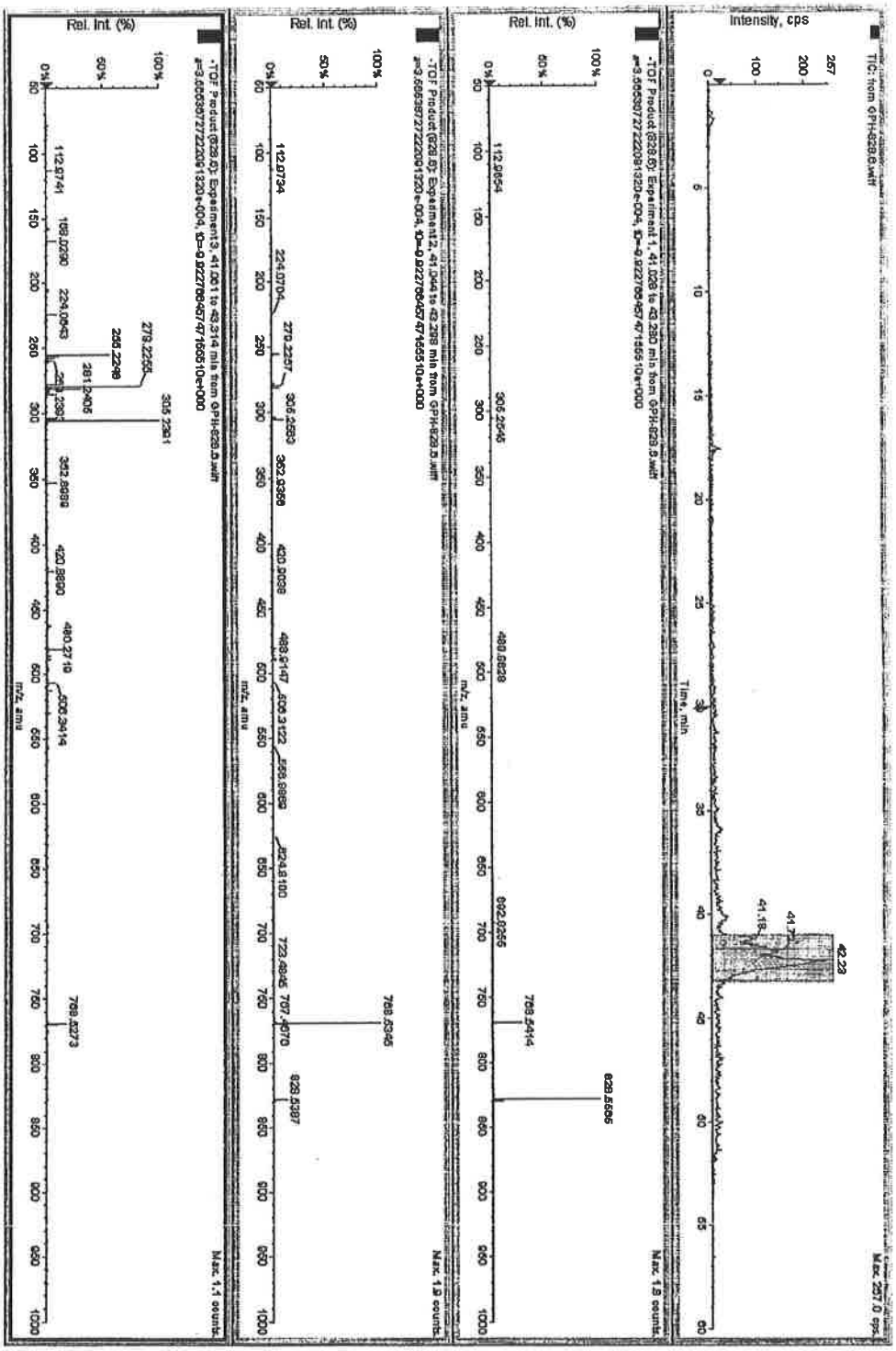

TIC from 6PH-628.0.wiff
Intensity, cps
Time, min
Max. 257.0 cps.
Max. 1.8 counts.
Rel. Int. (%)
m/z, amu
Max. 1.8 counts.
Rel. Int. (%)
m/z, amu
Max. 1.9 counts.
Rel. Int. (%)
m/z, amu
Max. 1.1 counts.

Figure 29

(a)

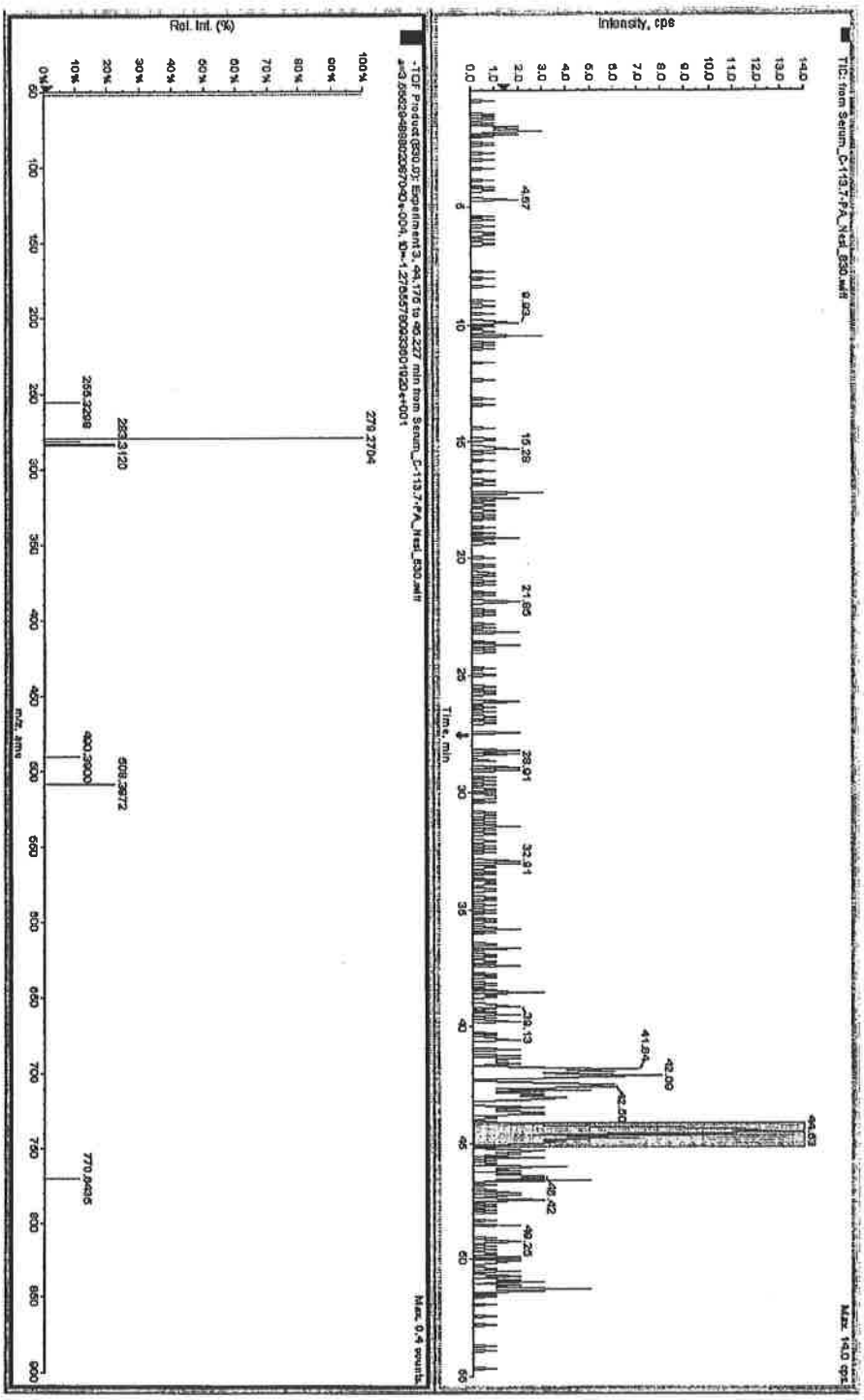

Intensity, cps
Time, min
Rel. Int. (%)
m/z, amu
279.2704
255.2299
283.3120
490.2900
509.3672
770.5435
41.54
42.00
42.50
44.63
46.42
49.25

Figure 30

(b)

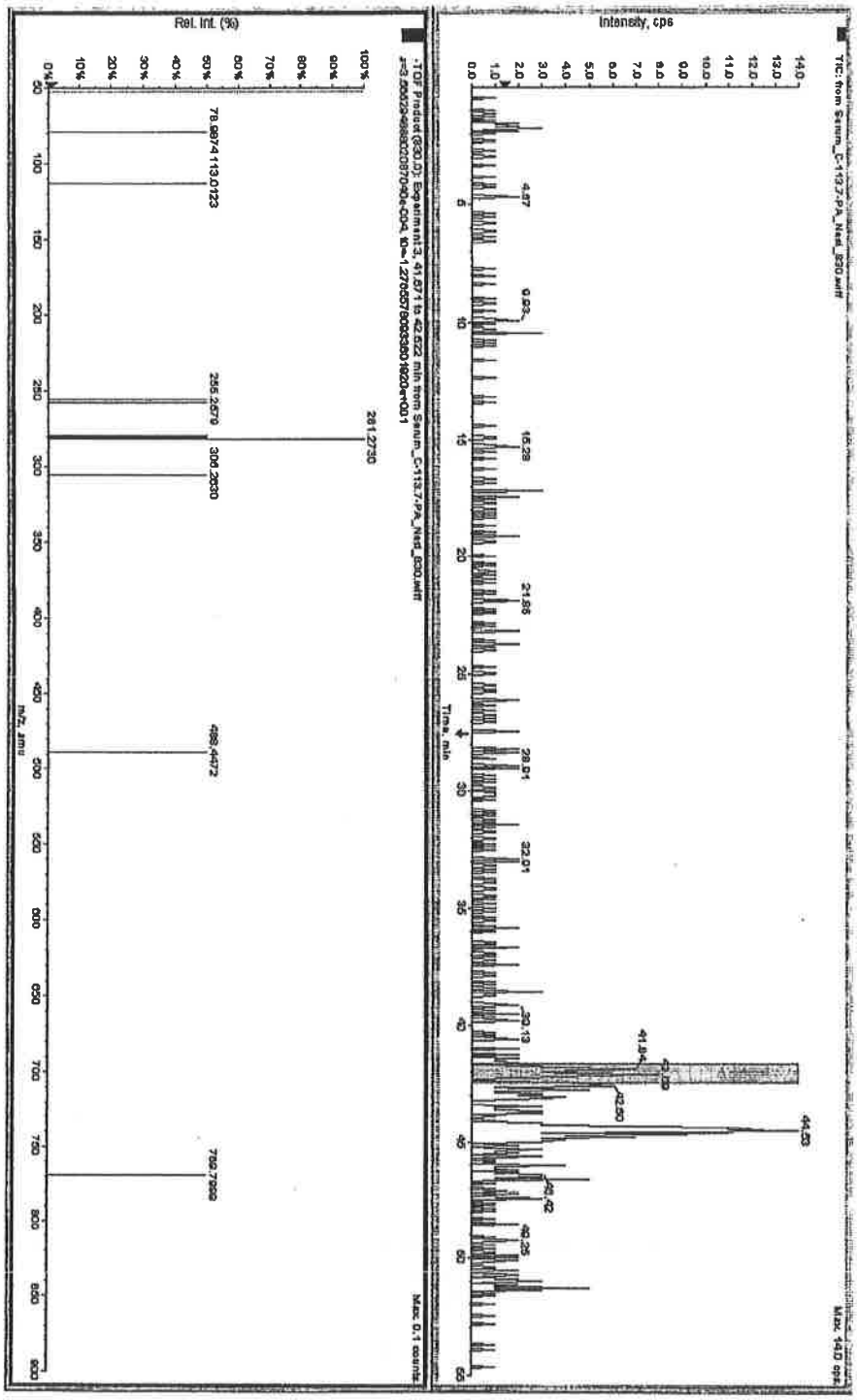


Figure 30 (cont.)

(a)

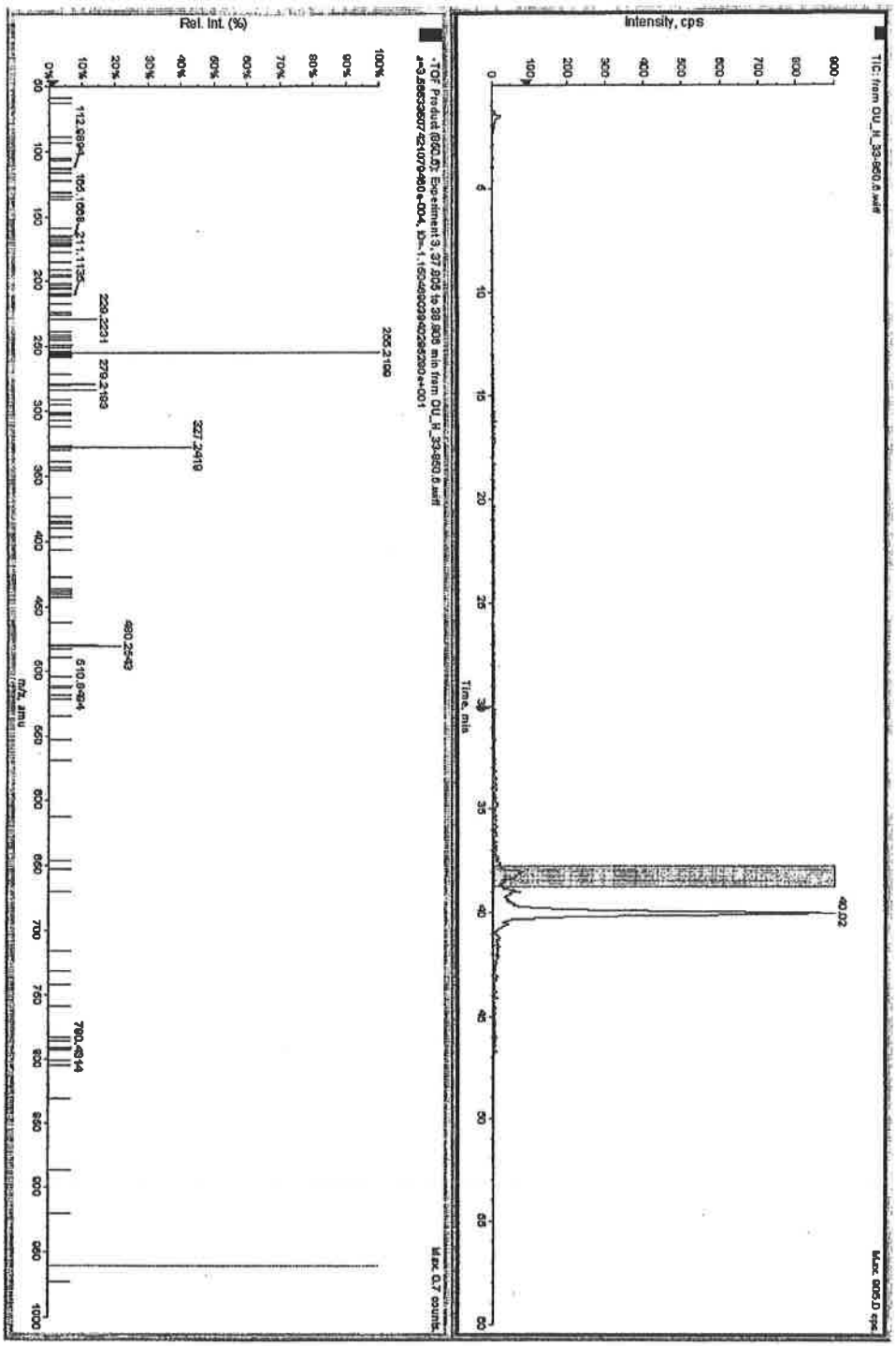

Intensity, cps
TIC: from OU_H_33-950.0.wiff
Max. 906.0 cps.
Time, min
40.02
Rel. Int. (%)
m/z, amu
Max. 0.7 counts
112.0894
105.1069
211.1135
229.2231
279.2193
305.2196
327.2419
480.2543
510.6494
790.4914

Figure 31

(b)

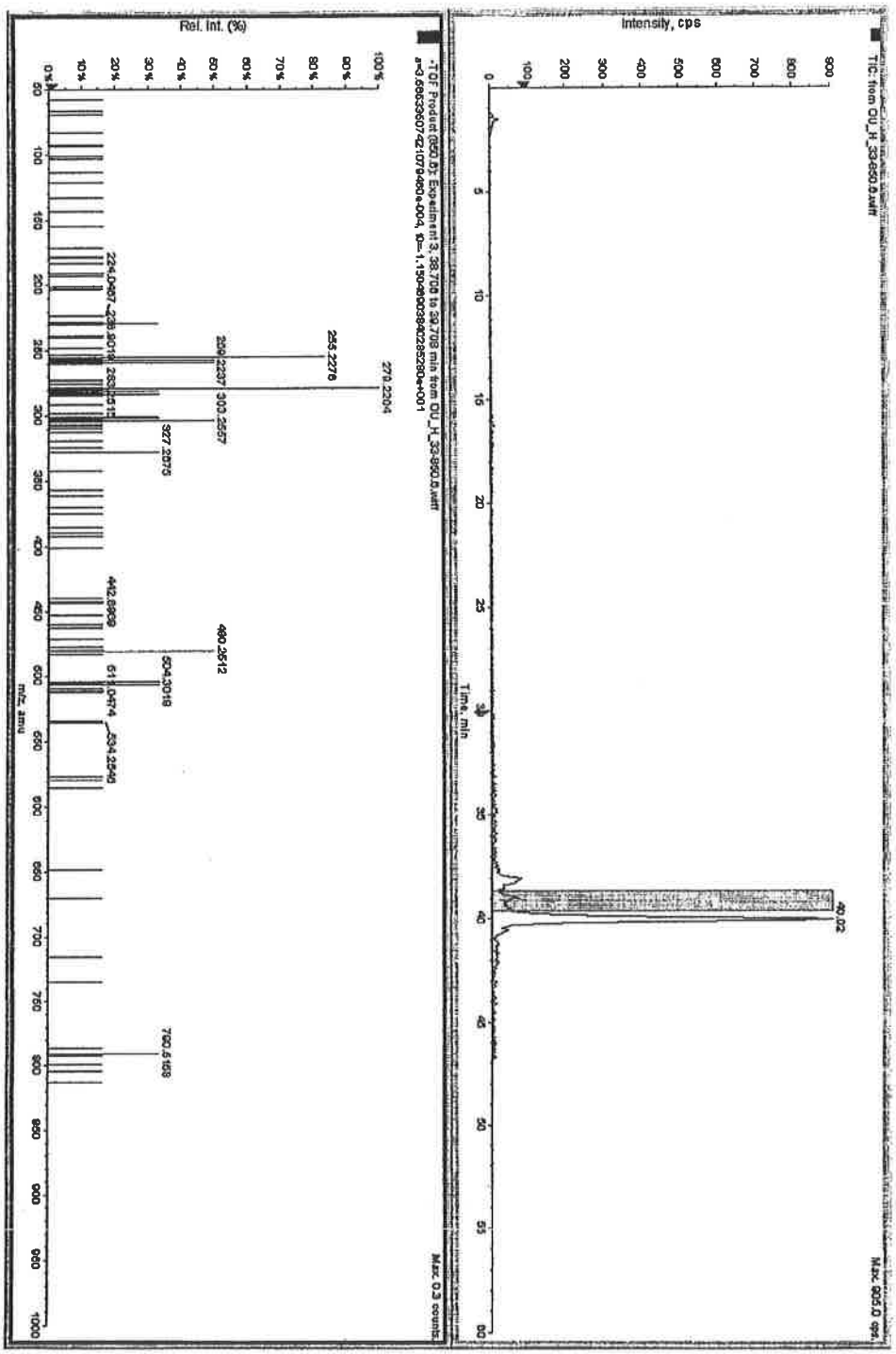


Figure 31 (cont.)

(c)

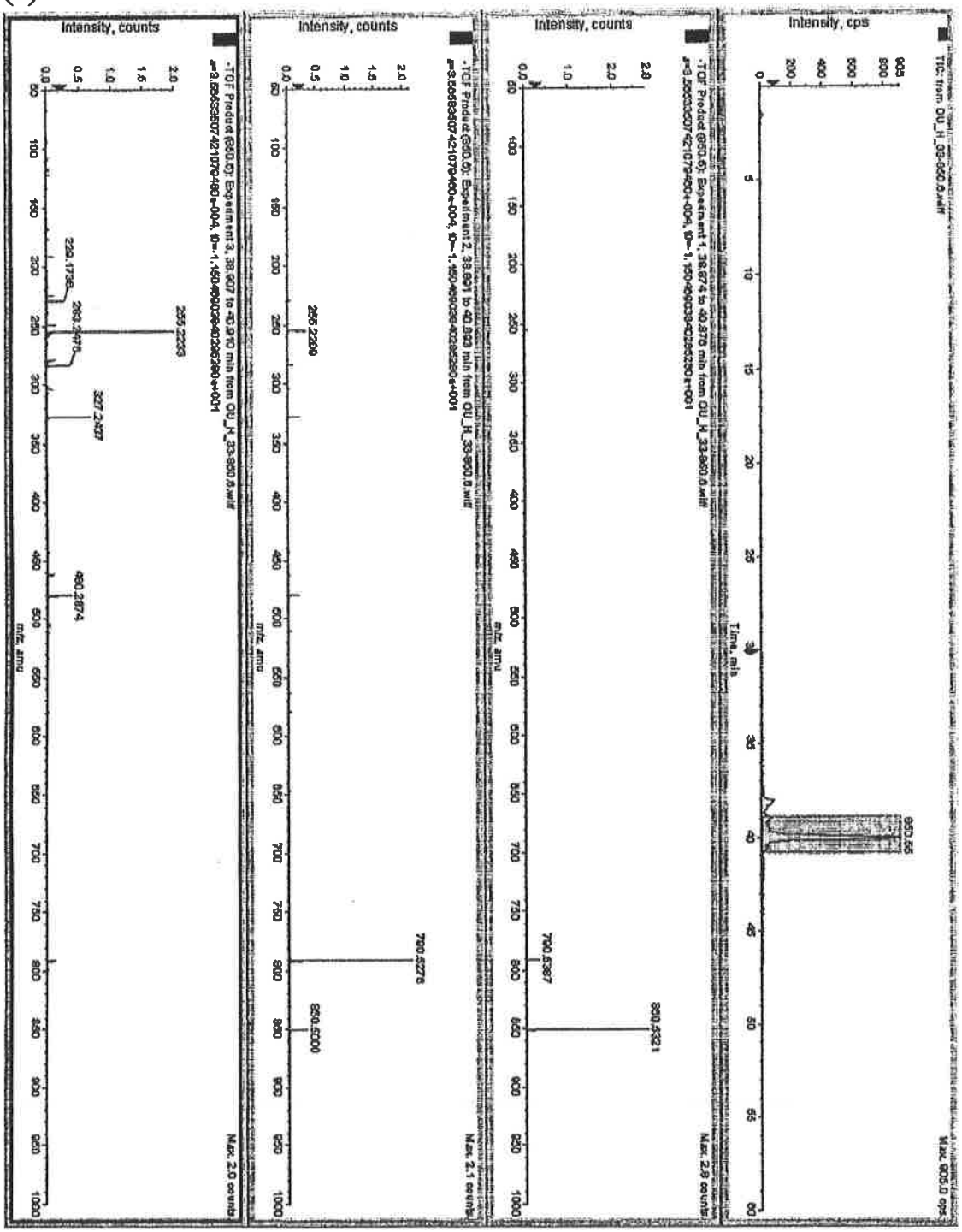


Figure 31 (cont.)

(d)

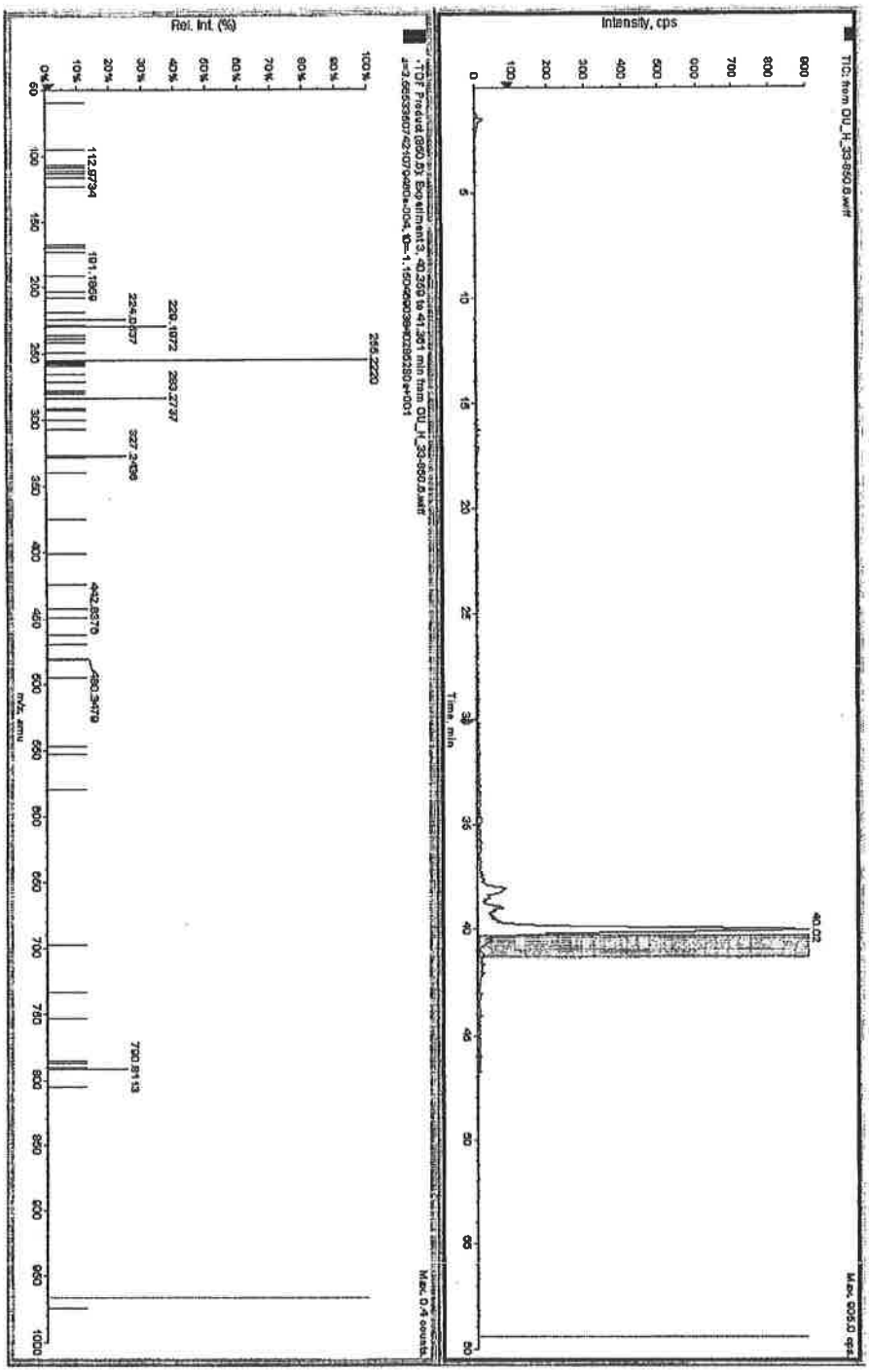


Figure 31 (cont.)

(a)

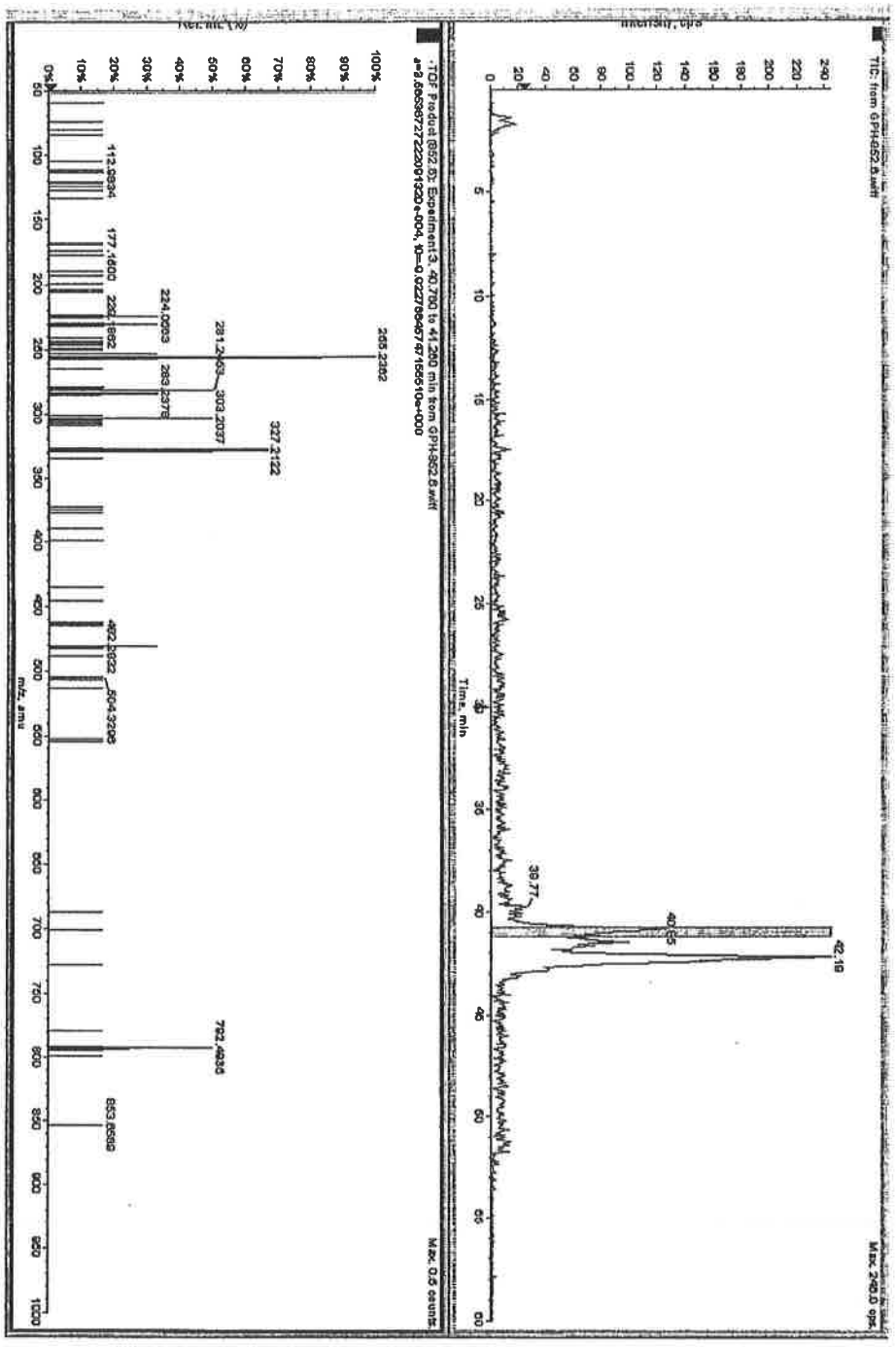

TIC: from GPH-862.6.wiff
Max. 248.0 cps.
Time, min
39.77
40.55
42.19
TOF Product (852.5): Experiment 3, 40.760 to 41.260 min from GPH-862.6.wiff
Max. 0.5 counts.
m/z, amu
112.9834
177.1600
224.0993
255.2382
281.2463
283.2378
303.2037
327.2122
492.3932
504.3206
792.4835
853.8569

Figure 32

(b)

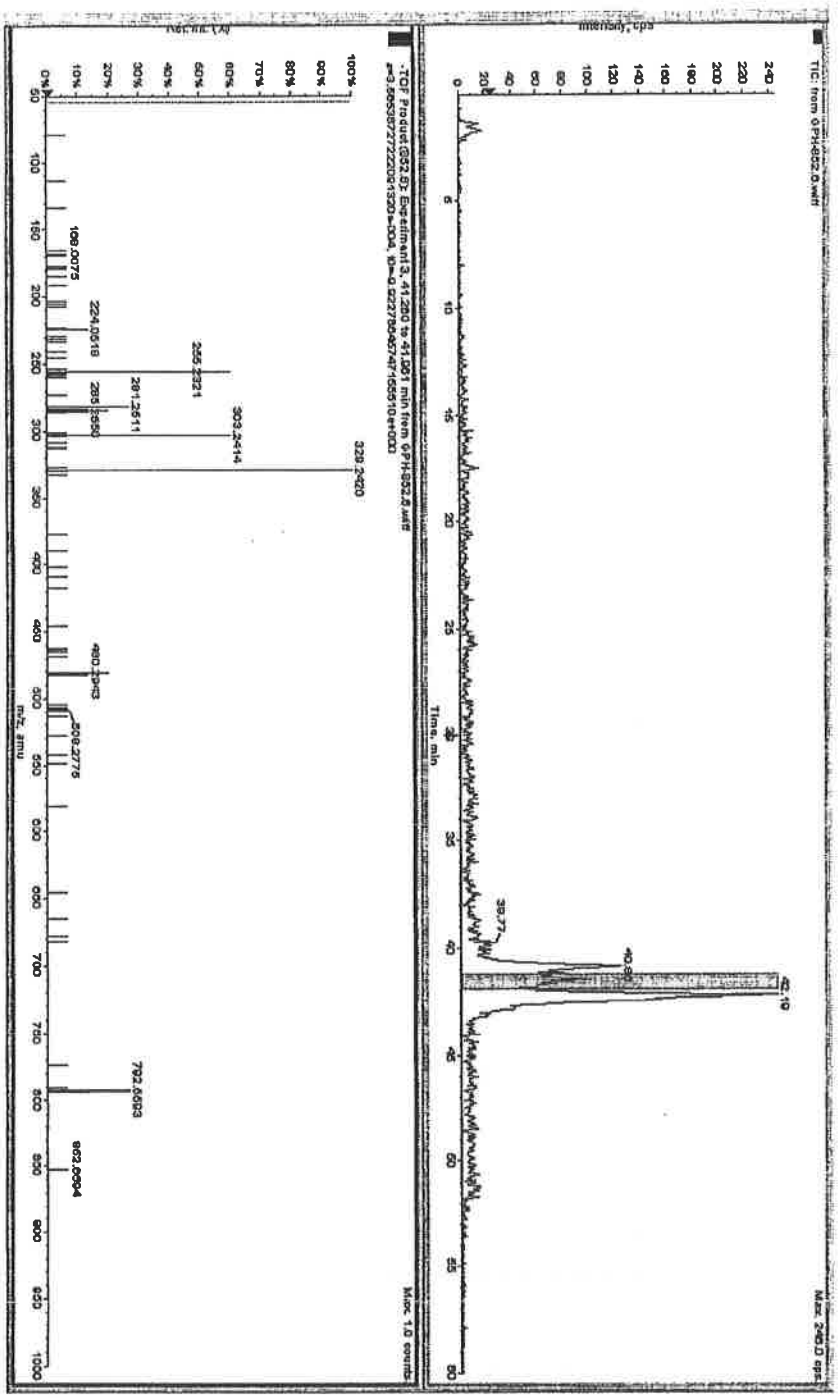


Figure 32 (cont.)

(c)

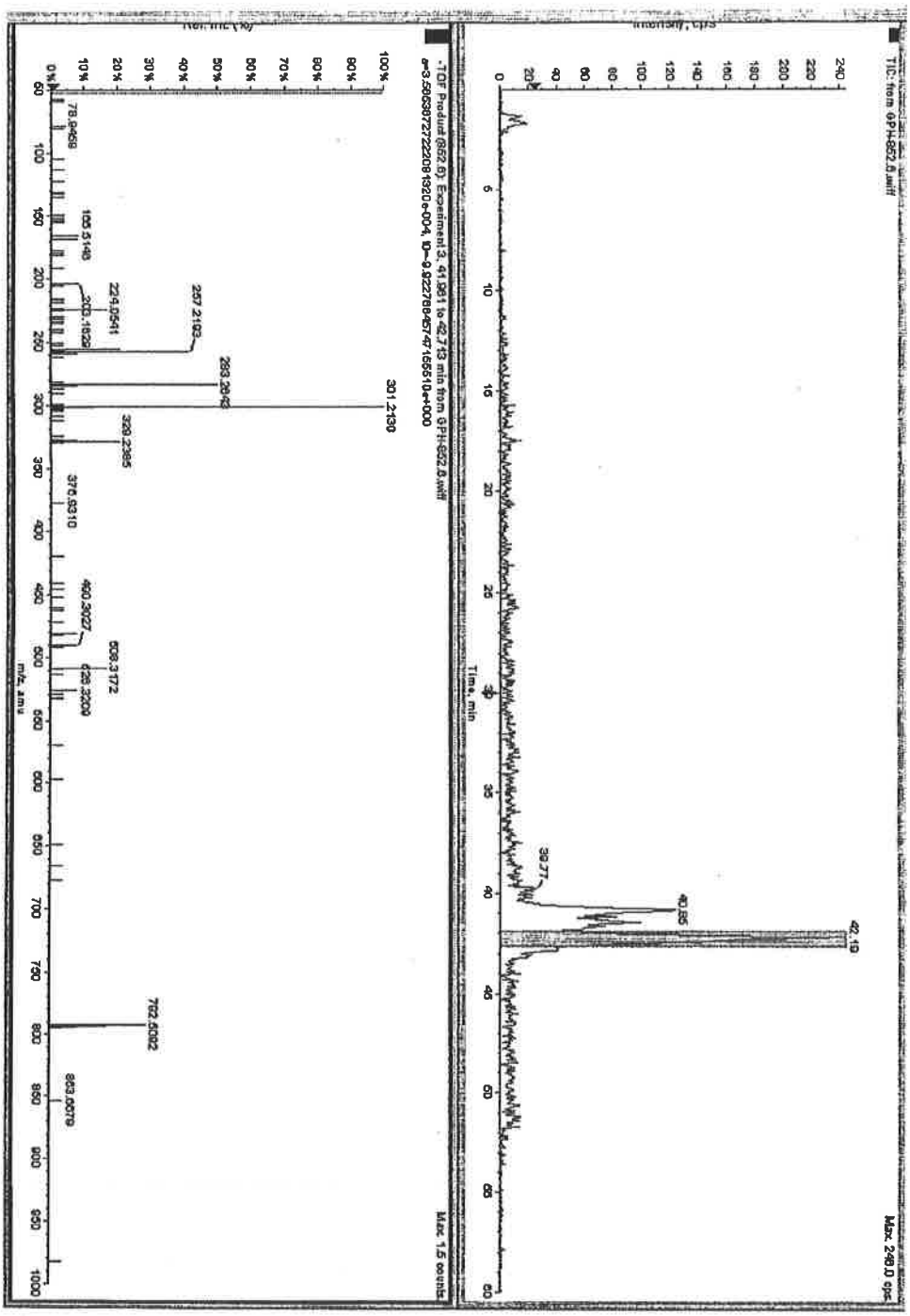


Figure 32 (cont.)

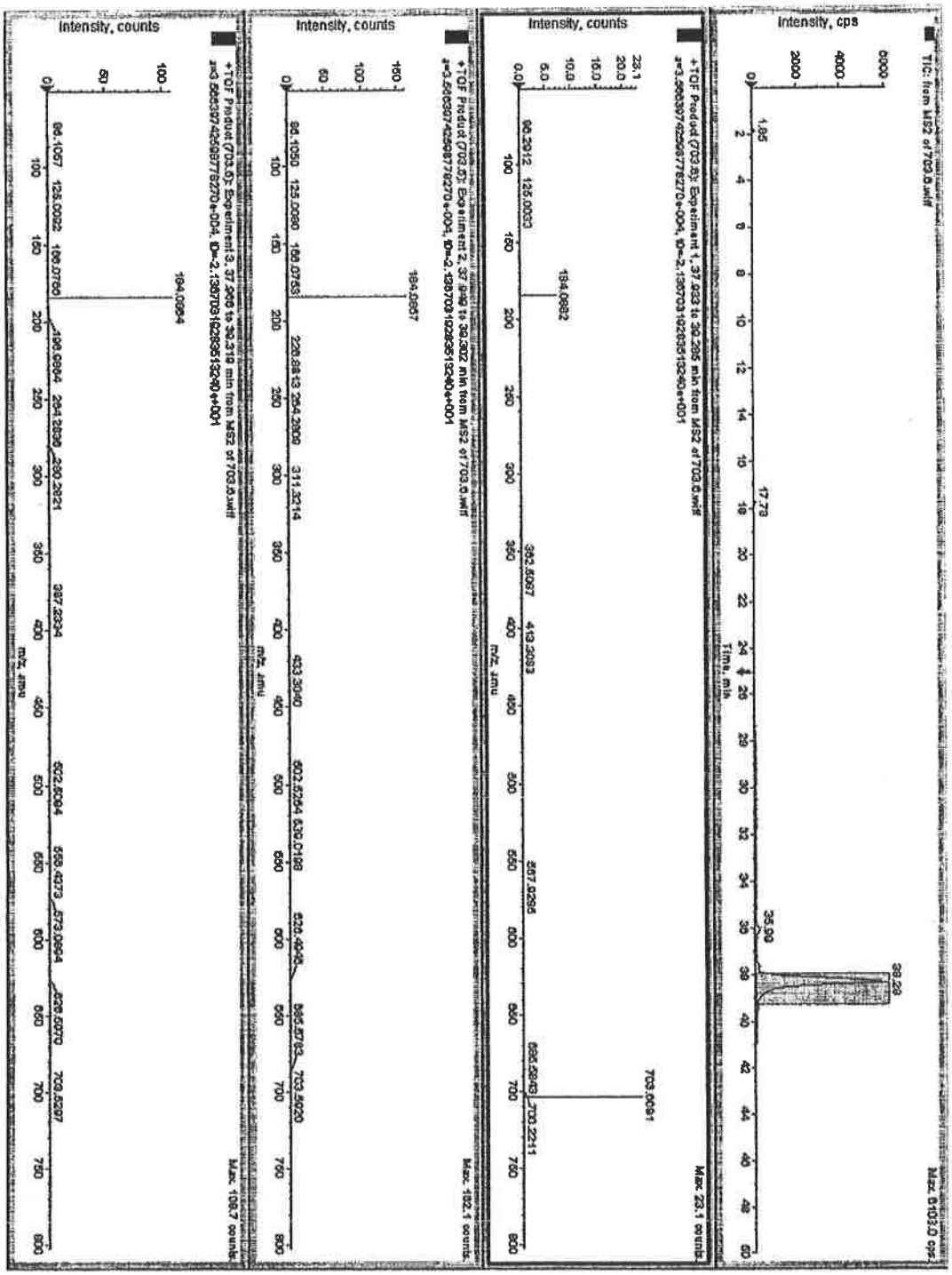

TIC: from MS2 of 703.5.wiff
Max: 6103.0 cps.
Intensity, cps
Time, min
1.85
17.73
35.99
38.23
+TOF Product (703.5): Experiment 1, 37.223 to 39.285 min from MS2 of 703.5.wiff
Max: 23.1 counts.
Intensity, counts
m/z, amu
98.3912
125.0033
194.0982
383.5097
413.2083
507.9295
586.5943
703.5091
700.2211
+TOF Product (703.5): Experiment 2, 37.649 to 39.302 min from MS2 of 703.5.wiff
Max: 192.1 counts.
Intensity, counts
m/z, amu
95.1050
125.0080
160.0755
194.0957
228.6813
254.2800
311.3214
433.3040
502.5264
530.0198
626.4648
666.8783
703.5020
+TOF Product (703.5): Experiment 3, 37.966 to 39.319 min from MS2 of 703.5.wiff
Max: 108.7 counts.
Intensity, counts
m/z, amu
96.1057
125.0092
160.0750
194.0954
196.9894
254.2826
280.2821
387.2334
502.5094
559.4073
573.0994
626.5070
703.5097

Figure 33

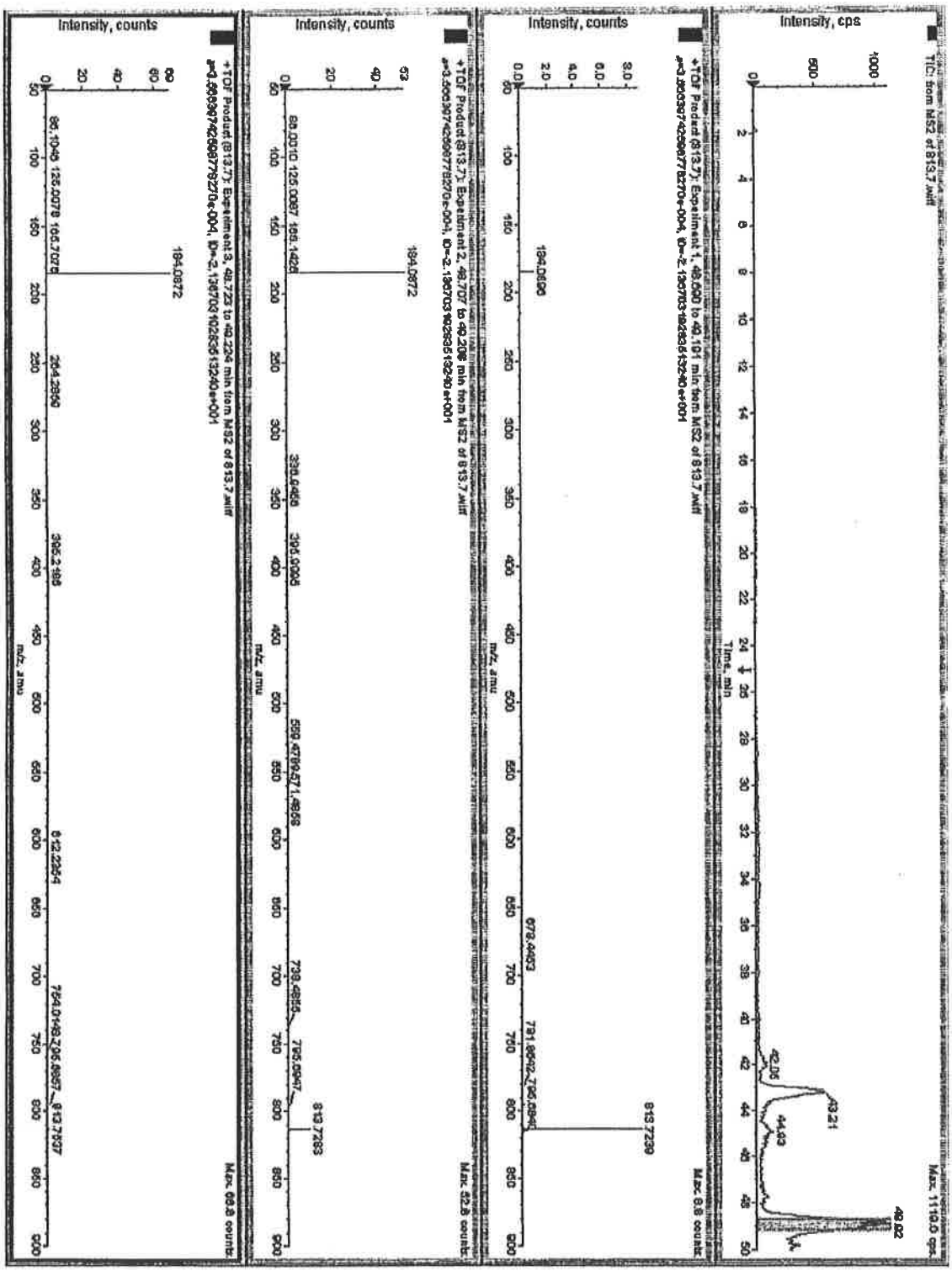

TIC: from MS2 of 813.7.wiff
Intensity, cps
Max. 1119.0 cps.
42.05
43.21
44.43
49.02
Time, min
+TOF Product (813.7): Experiment 1, 48.580 to 49.191 min from MS2 of 813.7.wiff
Intensity, counts
184.0696
678.4403
731.8642
813.7239
Max. 6.8 counts.
m/z, amu
+TOF Product (813.7): Experiment 2, 48.707 to 49.208 min from MS2 of 813.7.wiff
Intensity, counts
184.0672
330.6468
396.0005
550.4769
571.4858
738.4855
795.0947
813.7293
Max. 62.8 counts.
m/z, amu
+TOF Product (813.7): Experiment 3, 48.723 to 49.224 min from MS2 of 813.7.wiff
Intensity, counts
184.0672
86.1045
125.0078
165.7028
264.2850
396.2198
612.2254
754.0148
796.6857
813.7837
Max. 69.8 counts.
m/z, amu

Figure 34

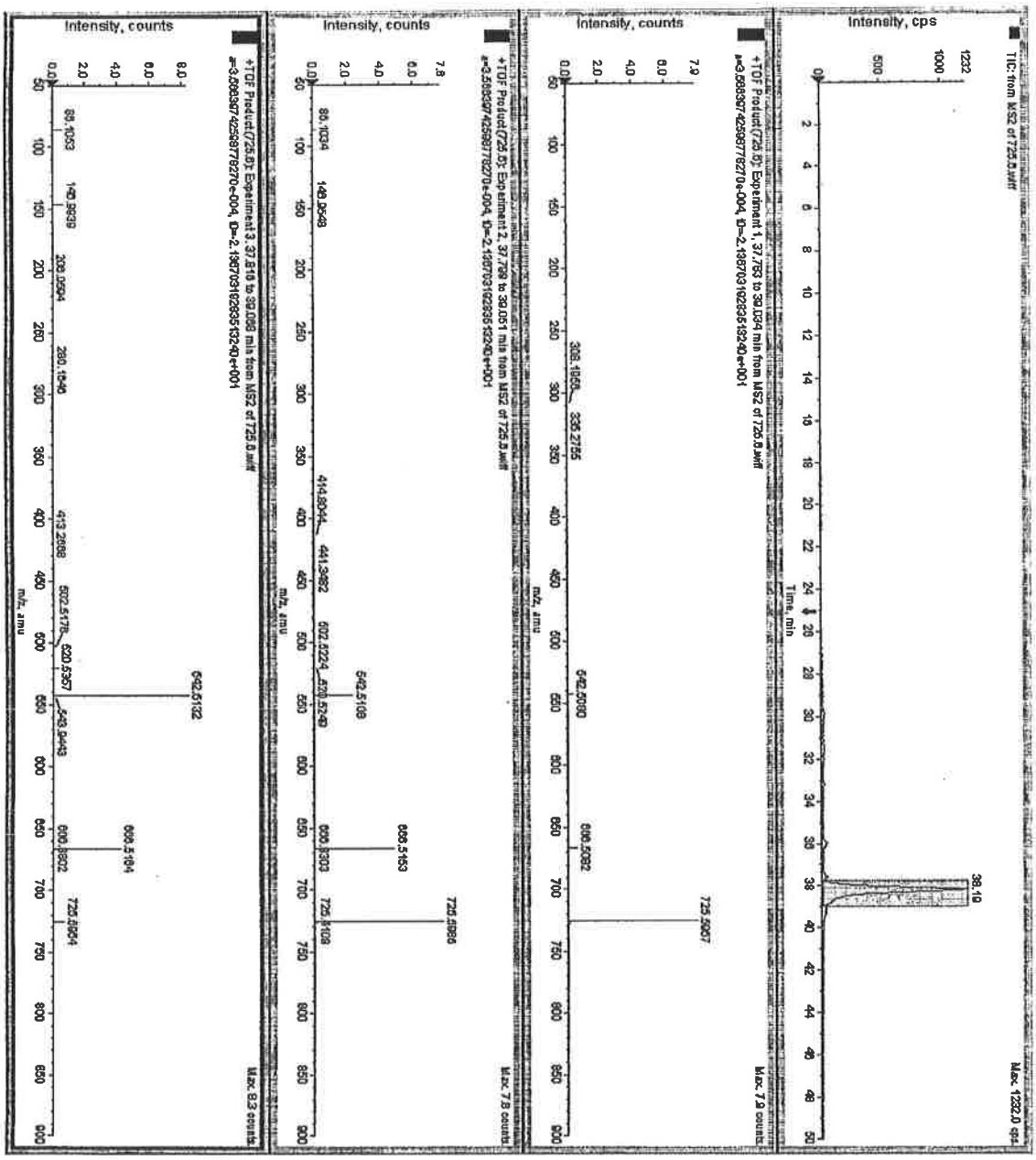

TIC: from MS2 of 725.5.wiff
Intensity, cps
Time, min
38.19
+TOF Product(725.5): Experiment 1, 37.783 to 39.034 min from MS2 of 725.5.wiff
Intensity, counts
m/z, amu
308.1956
338.2755
542.5090
606.5082
725.5067
+TOF Product(725.5): Experiment 2, 37.799 to 39.051 min from MS2 of 725.5.wiff
86.1034
149.0648
414.8044
441.2462
542.5108
602.5224
620.5249
668.5153
725.5926
+TOF Product(725.5): Experiment 3, 37.816 to 39.068 min from MS2 of 725.5.wiff
86.1053
149.0639
308.0594
260.1546
413.2688
502.5178
520.5357
542.5132
606.5164
725.5924
Max. 1232.0 cps.
Max. 79 counts.
Max. 83 counts.

Figure 35

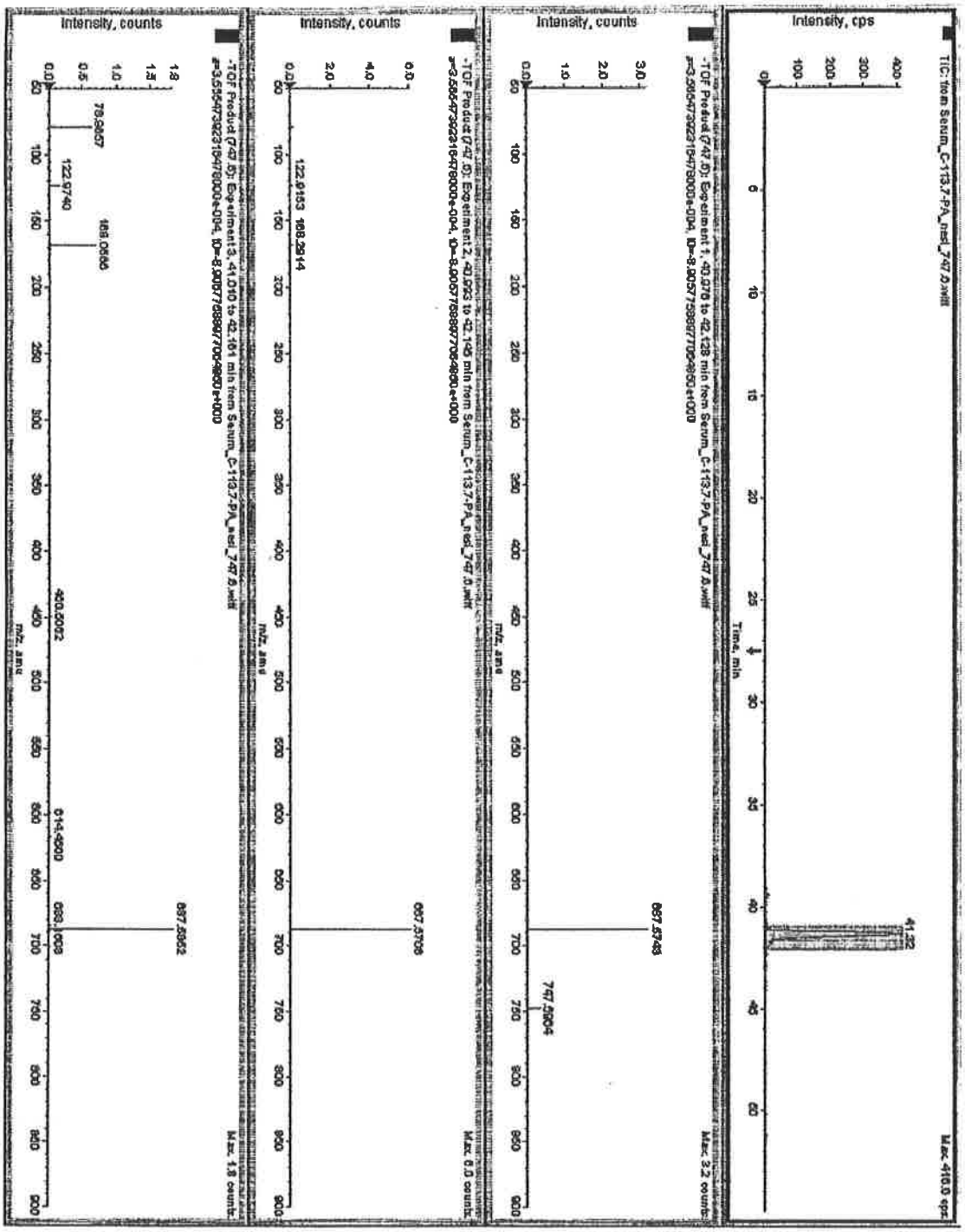

TIC: from Serum_C-113.7-PA_mel_747.0.wiff
Intensity, cps
Time, min
41.22
Max. 416.0 cps.
-TOF Product (747.0): Experiment 1, 40.976 to 42.128 min from Serum_C-113.7-PA_mel_747.0.wiff
Intensity, counts
m/z, amu
887.5748
747.5804
Max. 3.2 counts.
-TOF Product (747.0): Experiment 2, 40.993 to 42.145 min from Serum_C-113.7-PA_mel_747.0.wiff
Intensity, counts
m/z, amu
122.9153
168.2914
887.5708
Max. 6.0 counts.
-TOF Product (747.0): Experiment 3, 41.010 to 42.161 min from Serum_C-113.7-PA_mel_747.0.wiff
Intensity, counts
m/z, amu
78.9457
122.9740
168.0886
400.5092
614.4600
689.1008
887.5952
Max. 1.8 counts.

Figure 36

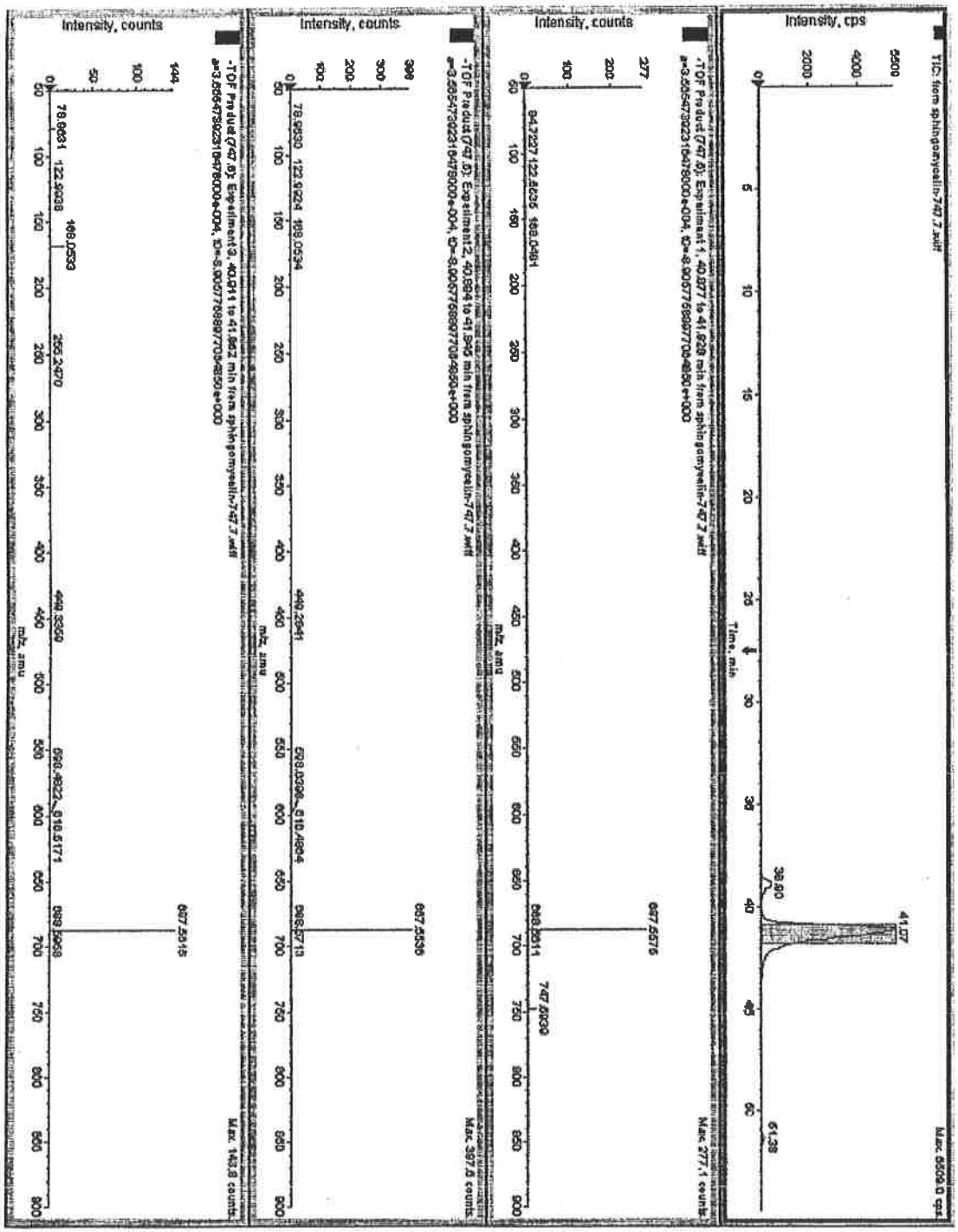

TIC: from sphingomyelin-747.7.wiff
Intensity, cps
Time, min
41.07
38.60
61.38
Max. 6506.0 cps.
-TOF Product (747.8): Experiment 1, 40.877 to 41.928 min from sphingomyelin-747.7.wiff
Intensity, counts
687.5575
747.6039
Max. 277.1 counts.
-TOF Product (747.8): Experiment 2, 40.894 to 41.945 min from sphingomyelin-747.7.wiff
687.5536
Max. 397.0 counts.
-TOF Product (747.8): Experiment 3, 40.911 to 41.962 min from sphingomyelin-747.7.wiff
687.5515
Max. 143.0 counts.
m/z, amu

Figure 37

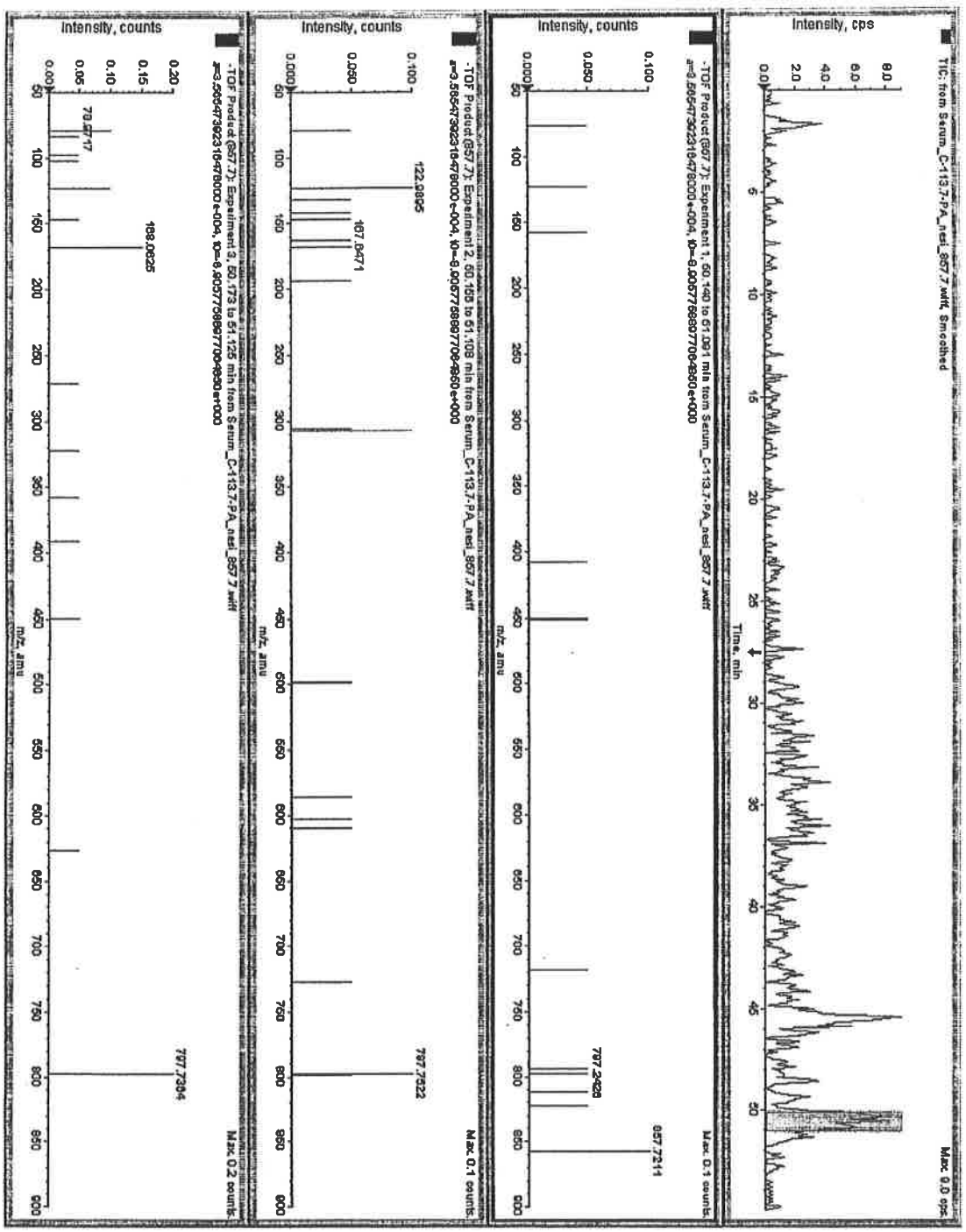

TIC: from Serum_C-113.7-PA_nesl_857.7.wiff, Smoothed
Intensity, cps
Max: 9.0 cps.
Time, min
Intensity, counts
-TOF Product (857.7): Experiment 1, 60.140 to 61.091 min from Serum_C-113.7-PA_nesl_857.7.wiff
Max: 0.1 counts.
857.7211
797.2426
m/z, amu
Intensity, counts
-TOF Product (857.7): Experiment 2, 60.159 to 61.109 min from Serum_C-113.7-PA_nesl_857.7.wiff
Max: 0.1 counts.
122.0925
167.8471
797.7522
m/z, amu
Intensity, counts
-TOF Product (857.7): Experiment 3, 60.173 to 61.125 min from Serum_C-113.7-PA_nesl_857.7.wiff
Max: 0.2 counts.
79.5717
169.0825
797.7384
m/z, amu

Figure 38

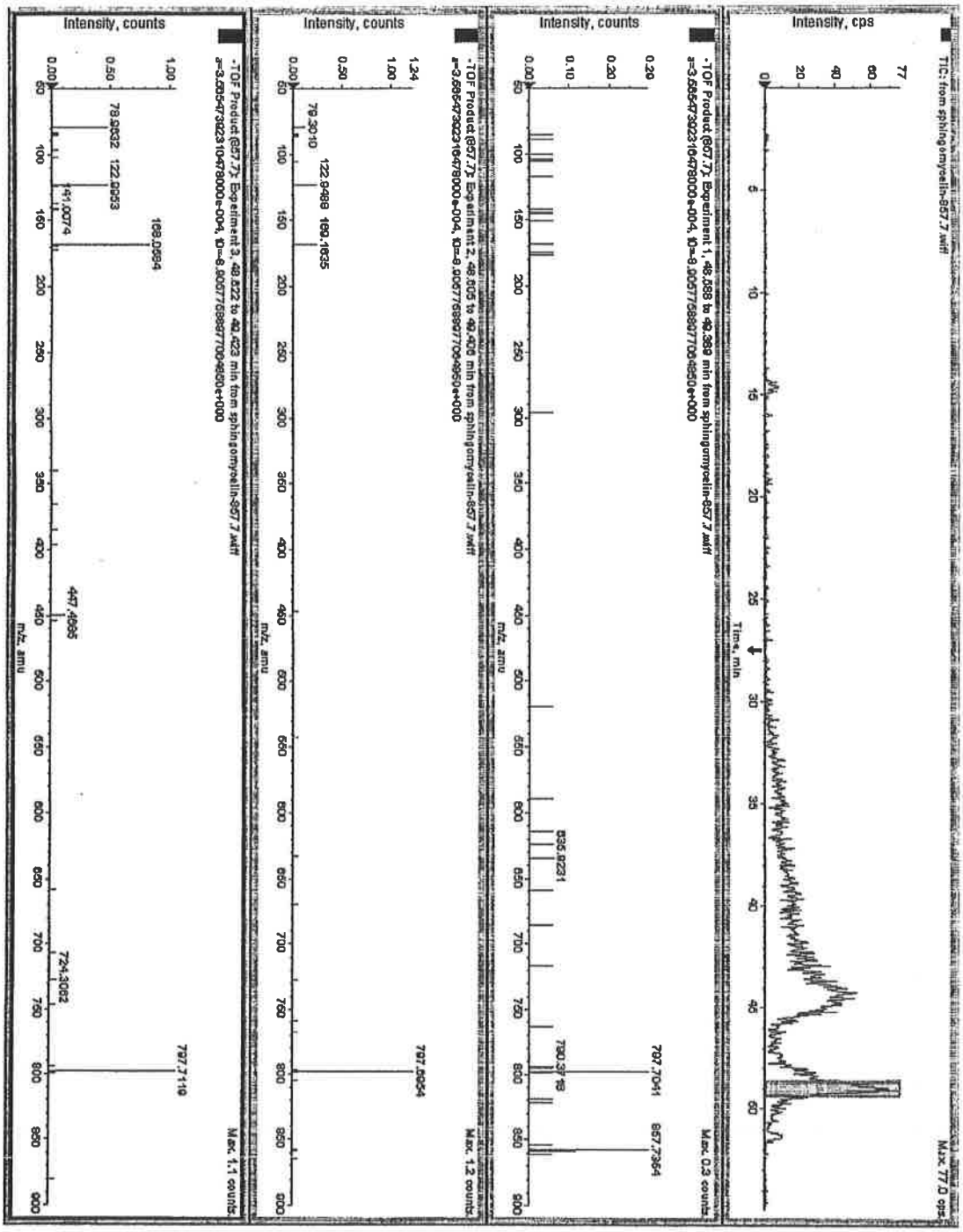

Intensity, cps
TIC: from sphingomyelin-857.7.wiff
Max. 77.0 cps.
Time, min
Intensity, counts
- TOF Product (857.7): Experiment 1, 48.588 to 49.369 min from sphingomyelin-857.7.wiff
Max. 0.3 counts.
535.9231
730.3718
797.7041
857.7364
m/z, amu
Intensity, counts
- TOF Product (857.7): Experiment 2, 48.005 to 49.406 min from sphingomyelin-857.7.wiff
Max. 1.2 counts.
79.3010
122.9498
169.1635
797.5934
m/z, amu
Intensity, counts
- TOF Product (857.7): Experiment 3, 48.822 to 49.423 min from sphingomyelin-857.7.wiff
Max. 1.1 counts.
79.9632
122.0953
169.0994
141.0074
447.4696
724.3062
797.7119
m/z, amu

Figure 39

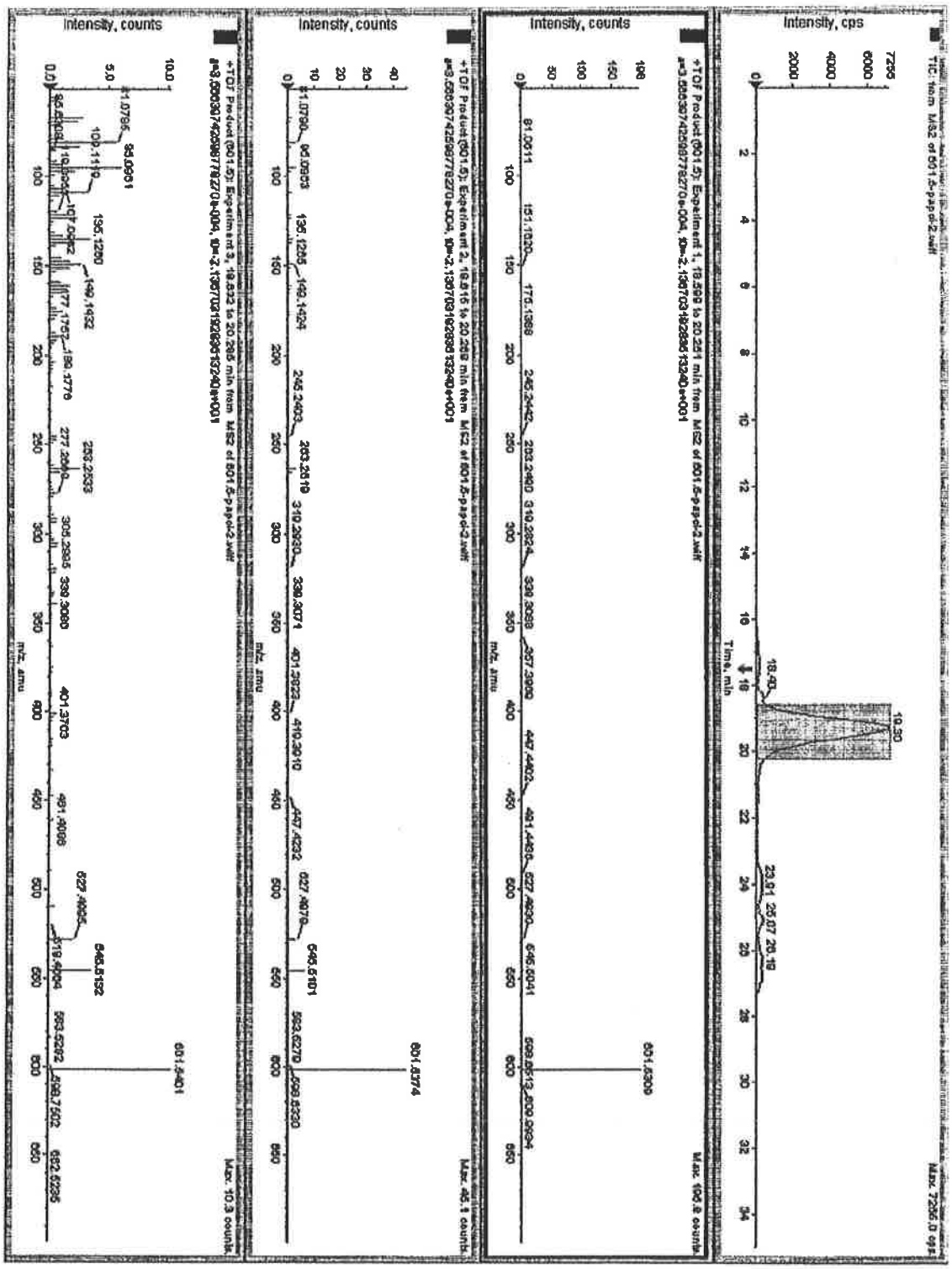
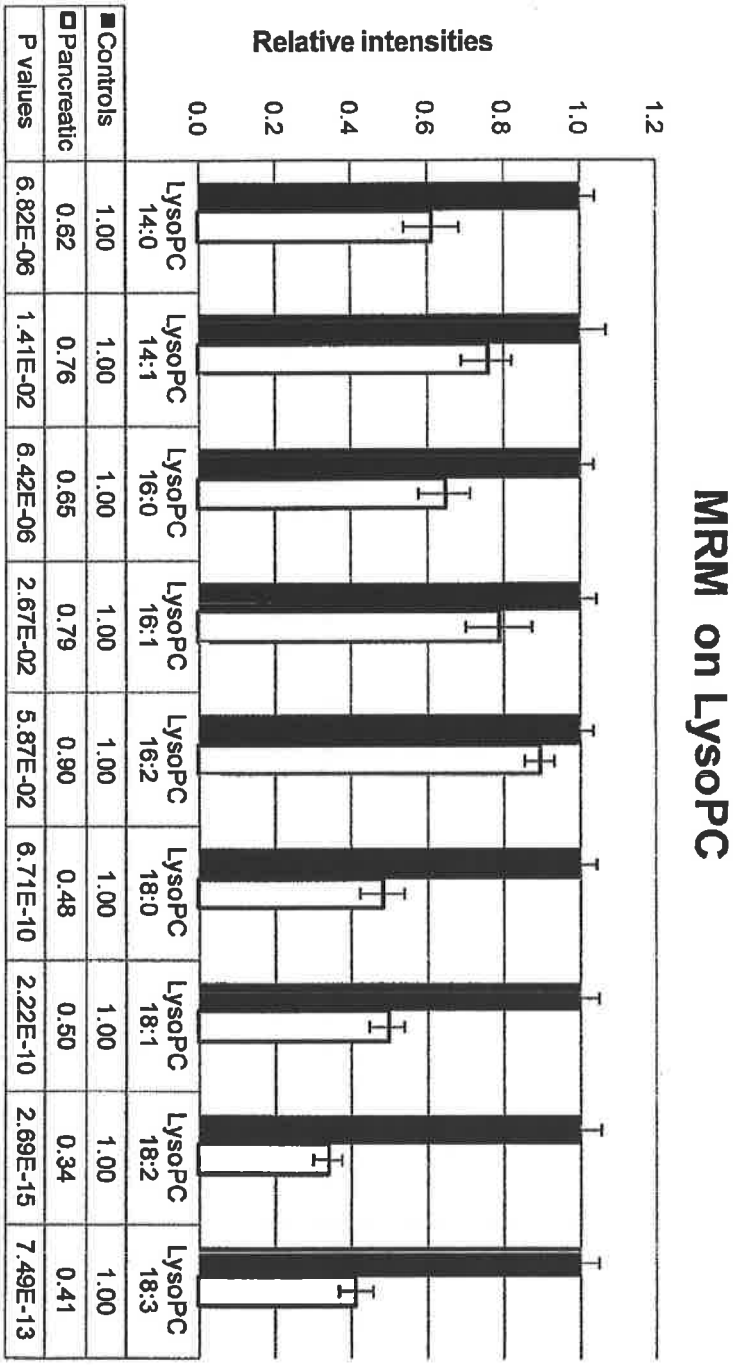

Intensity, cps
Time, min
18.43
19.30
23.01
25.07
26.19
Intensity, counts
m/z, amu
601.5300
Intensity, counts
m/z, amu
601.5374
Intensity, counts
m/z, amu
601.5401

Figure 40

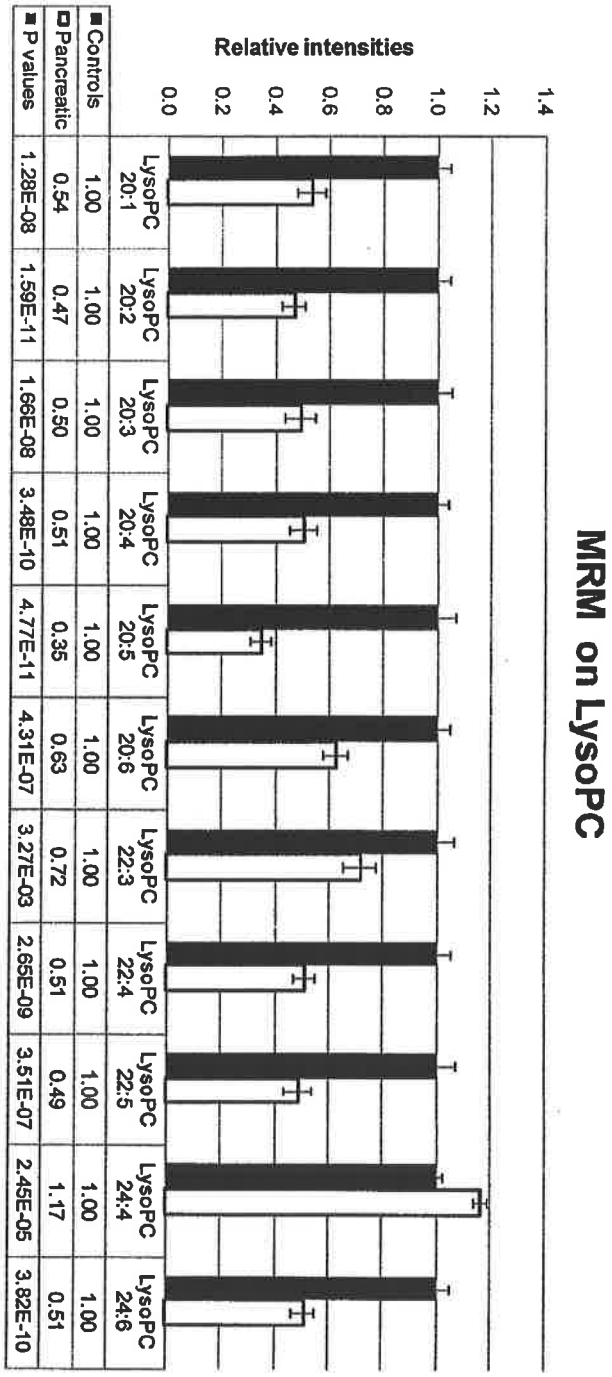
(a)



	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

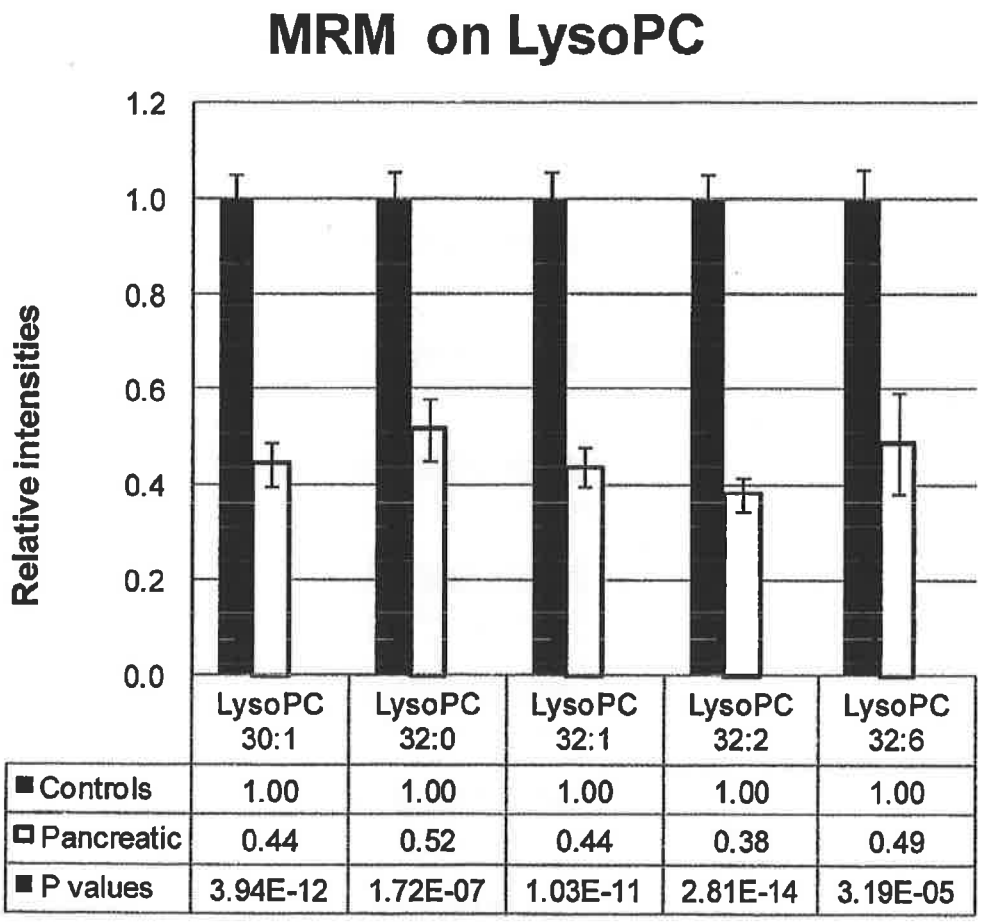
(b)



	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.)

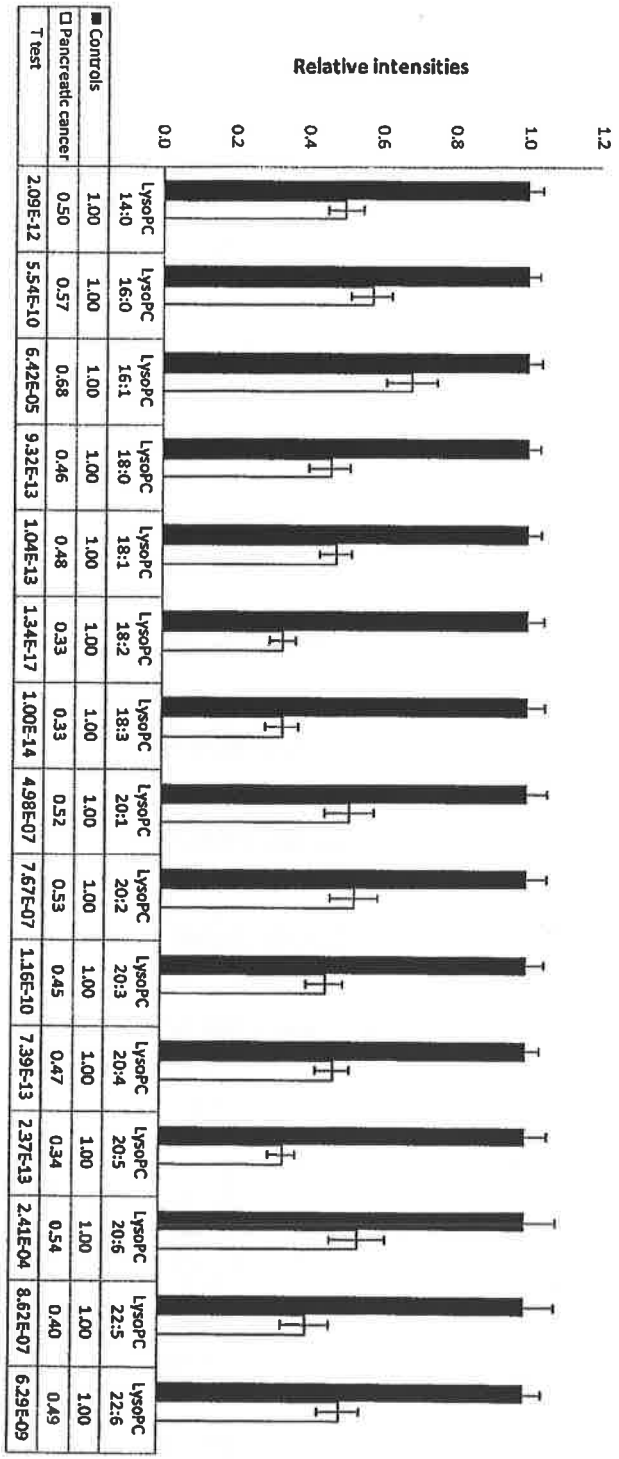
(c)



	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.)

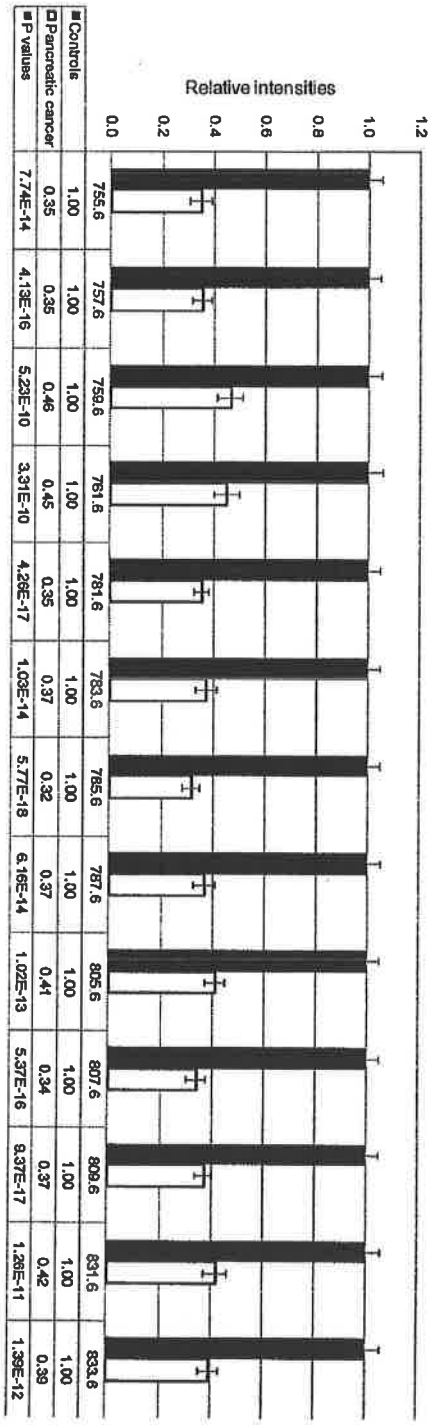
(d)



	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
T 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.)

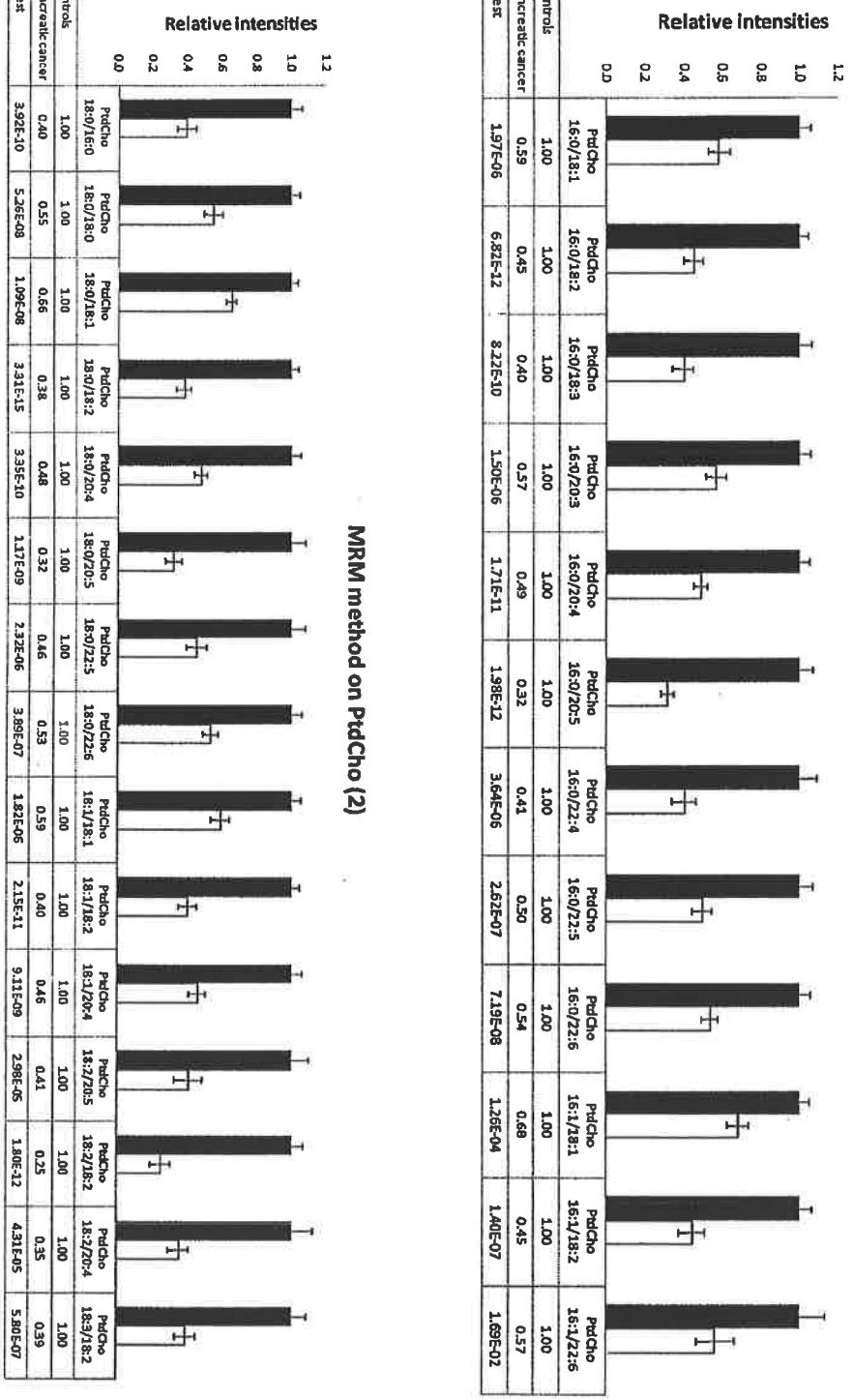
a)



	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)

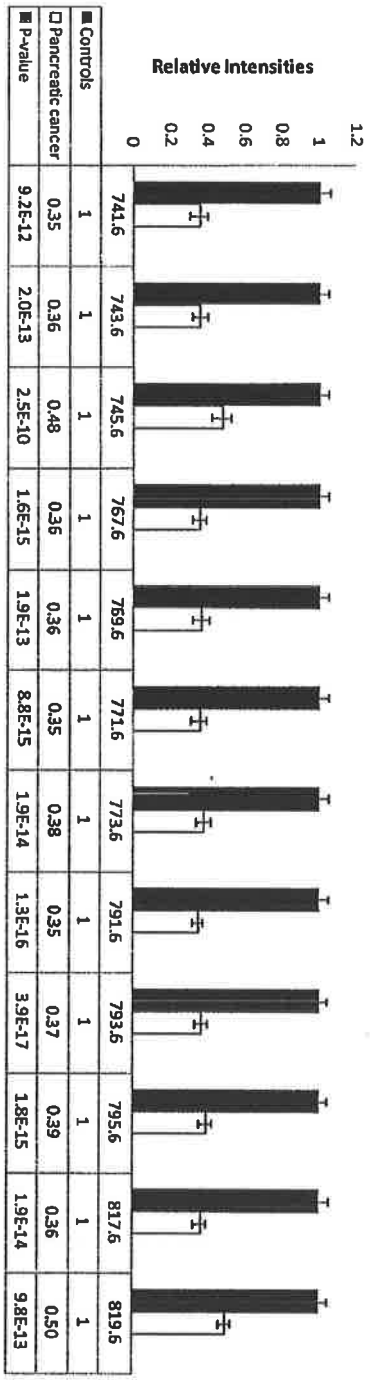


	PtdCho 16:0/18:1	PtdCho 16:0/18:2	PtdCho 16:0/18:3	PtdCho 16:0/20:3	PtdCho 16:0/20:4	PtdCho 16:0/20:5	PtdCho 16:0/22:4	PtdCho 16:0/22:5	PtdCho 16:0/22:6	PtdCho 16:1/18:1	PtdCho 16:1/18:2	PtdCho 16:1/22:6
■ Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
□ Pancreatic cancer	0.59	0.45	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

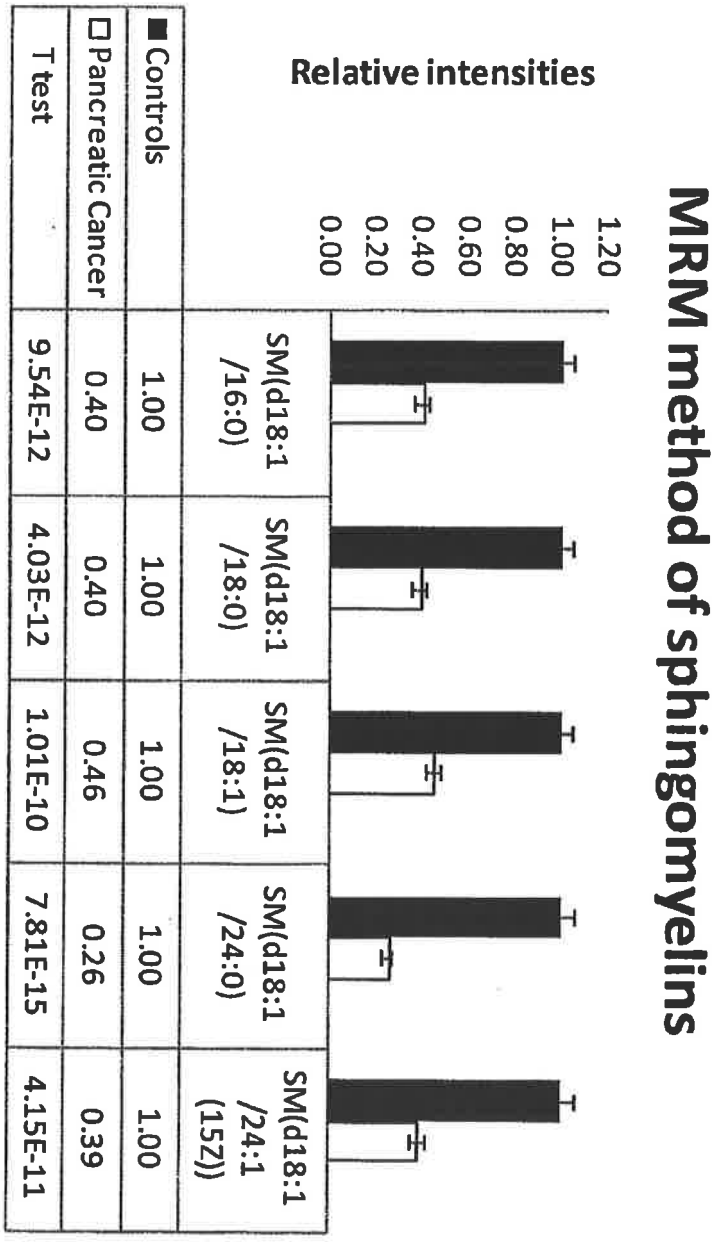
Figure 42 (cont.)

c)



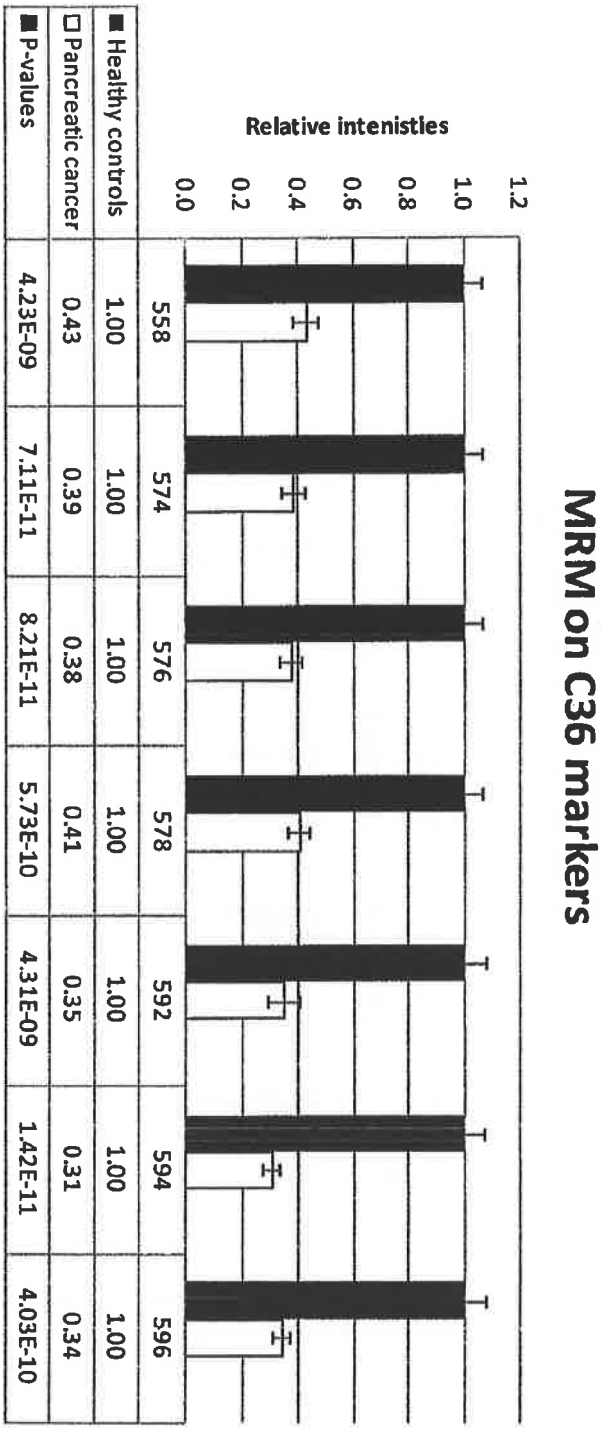
	741.6	743.6	745.6	767.6	769.6	771.6	773.6	791.6	793.6	795.6	817.6	819.6
■ Controls	1	1	1	1	1	1	1	1	1	1	1	1
□ Pancreatic cancer	0.35	0.36	0.48	0.36	0.36	0.35	0.38	0.35	0.37	0.39	0.36	0.50
■ P-value	9.2E-12	2.0E-13	2.5E-10	1.6E-15	1.9E-13	8.8E-15	1.9E-14	1.3E-16	3.9E-17	1.8E-15	1.9E-14	9.8E-13

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

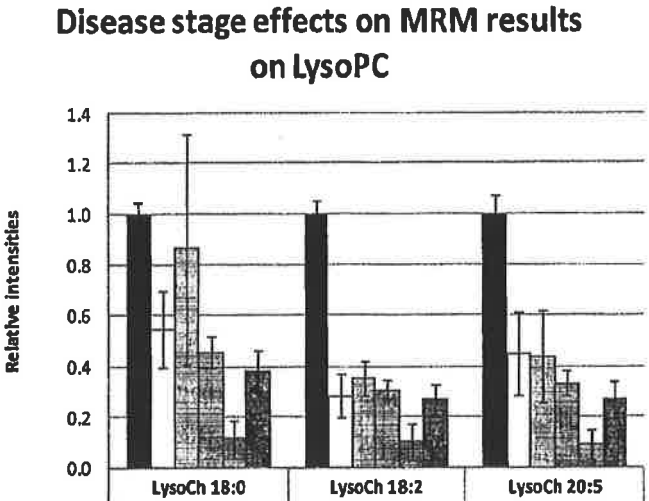
Figure 43



	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

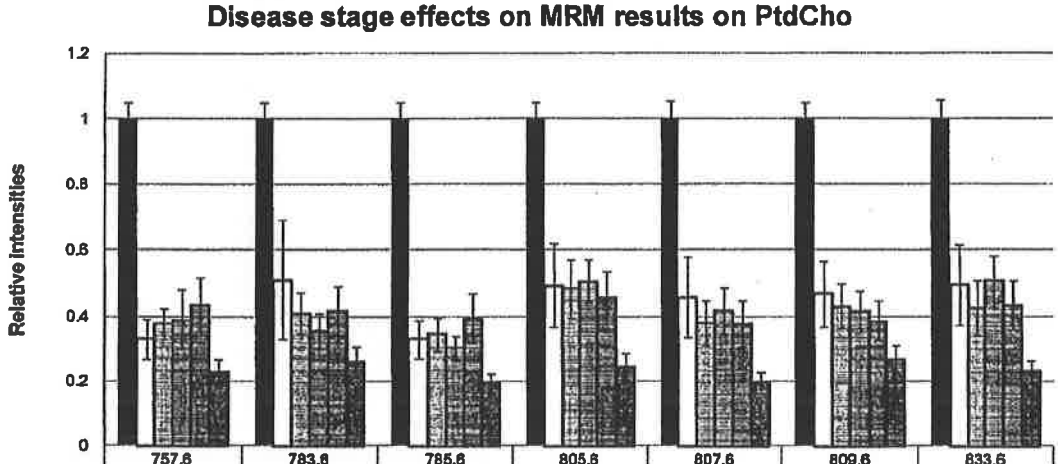
Figure 44

(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

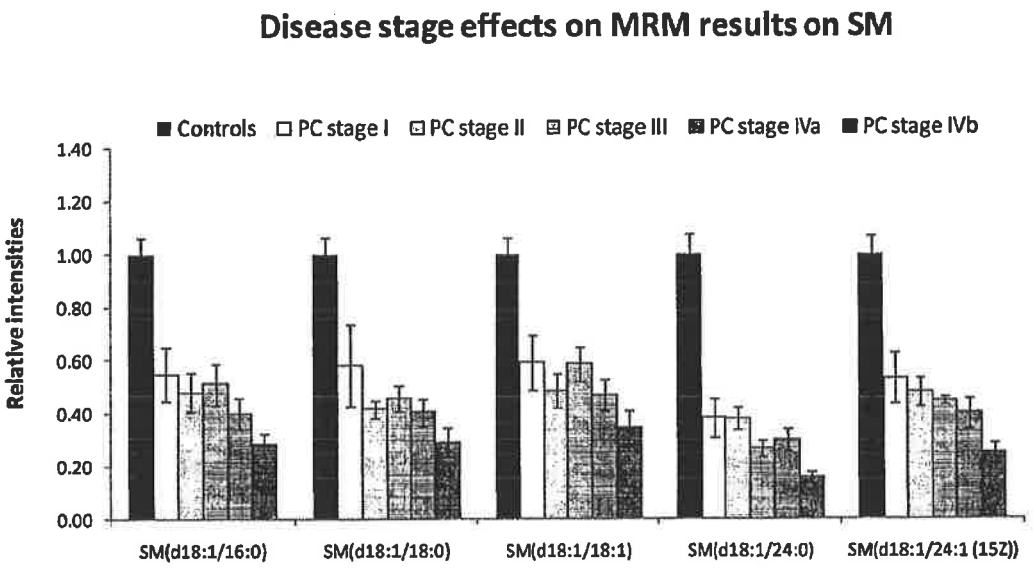
(b)



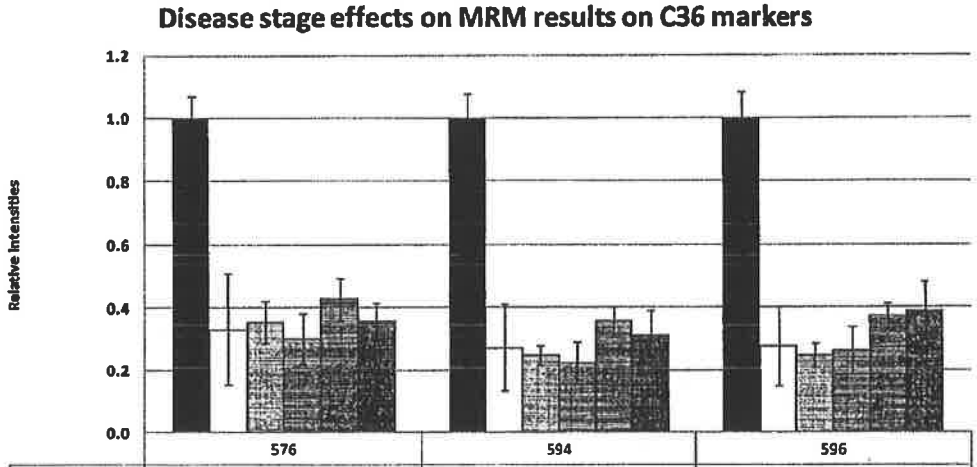
	757.6	783.6	785.6	805.6	807.6	809.6	833.6
Controls	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Stage I	0.33	0.51	0.33	0.49	0.46	0.47	0.50
Stage II	0.38	0.41	0.34	0.48	0.38	0.43	0.43
Stage III	0.39	0.35	0.30	0.51	0.42	0.42	0.51
Stage IVa	0.43	0.42	0.39	0.46	0.38	0.39	0.43
Stage IVb	0.22	0.26	0.19	0.24	0.19	0.27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

Figure 45

(c)



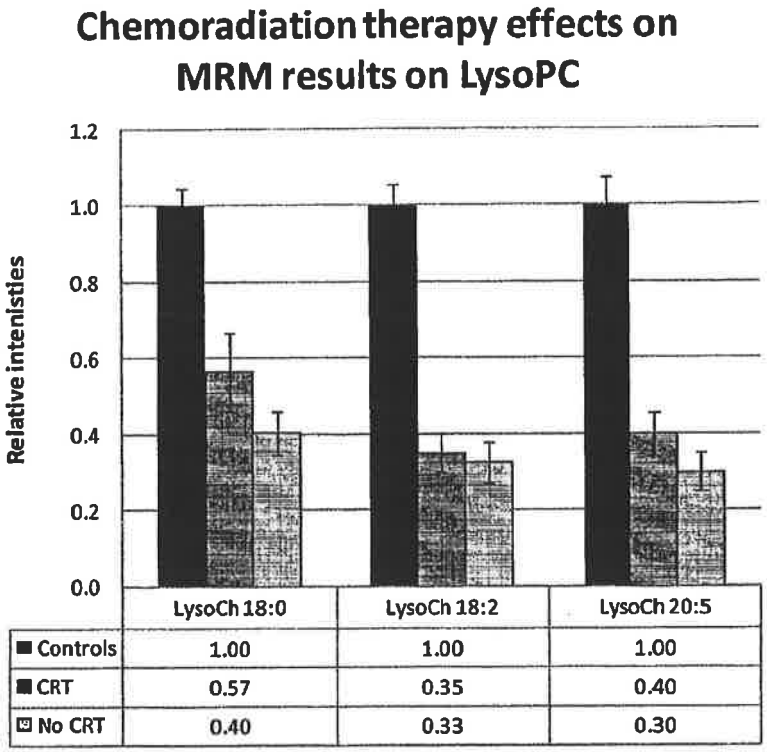
(d)



	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

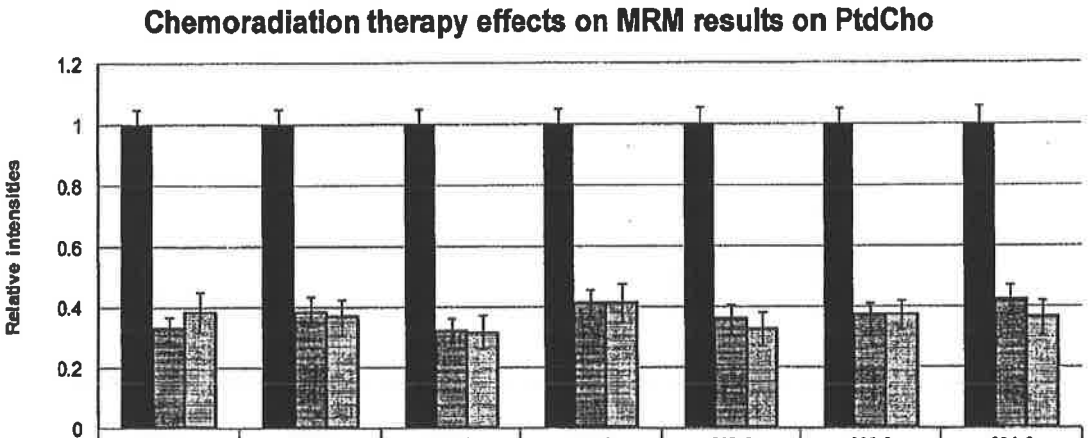
Figure 45 (Cont.)

(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

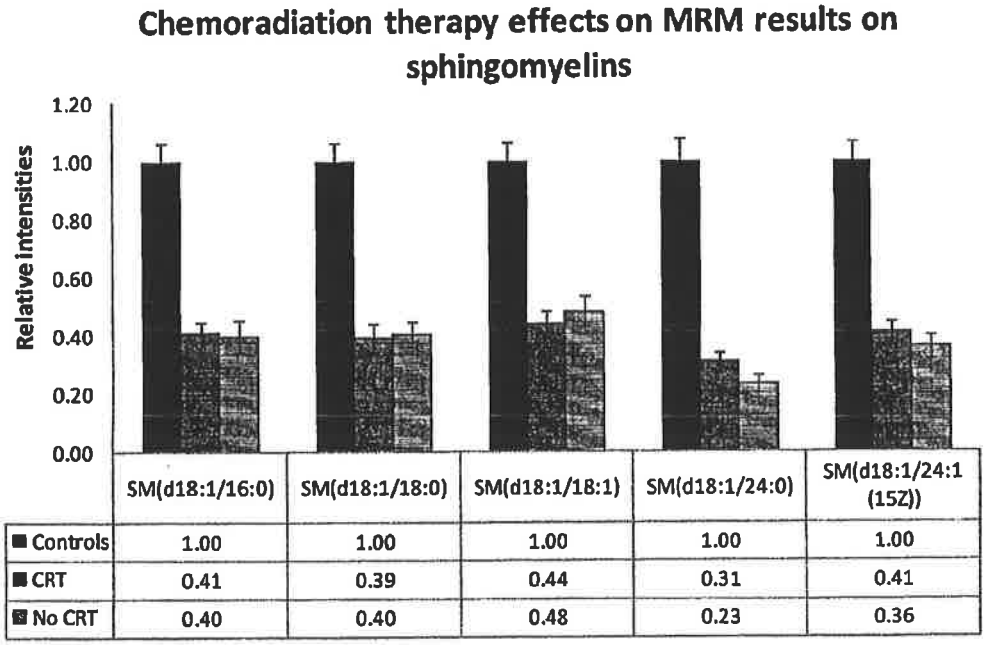
(b)



	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

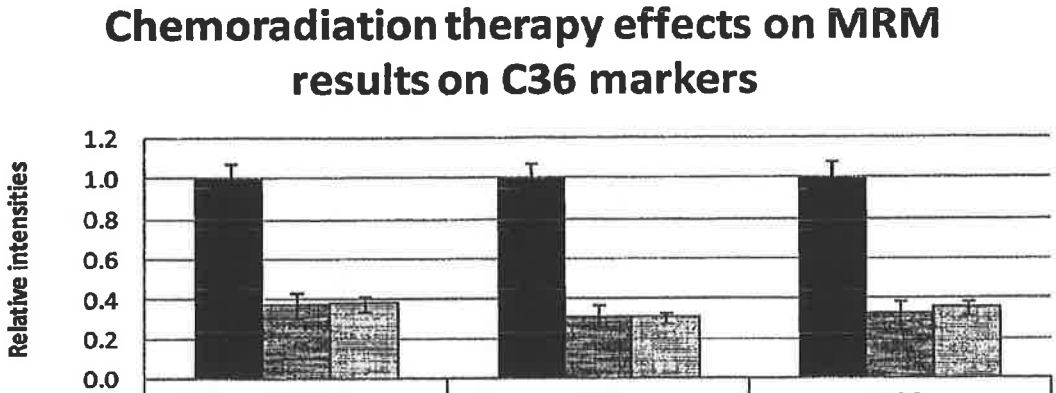
Figure 46

(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.)