Supplementary Material

Phosphorylation of 10-bromoanthracen-9-yl-cyclopenta[*d*]isoxazol-6-ols: chemistry suitable for antivirals

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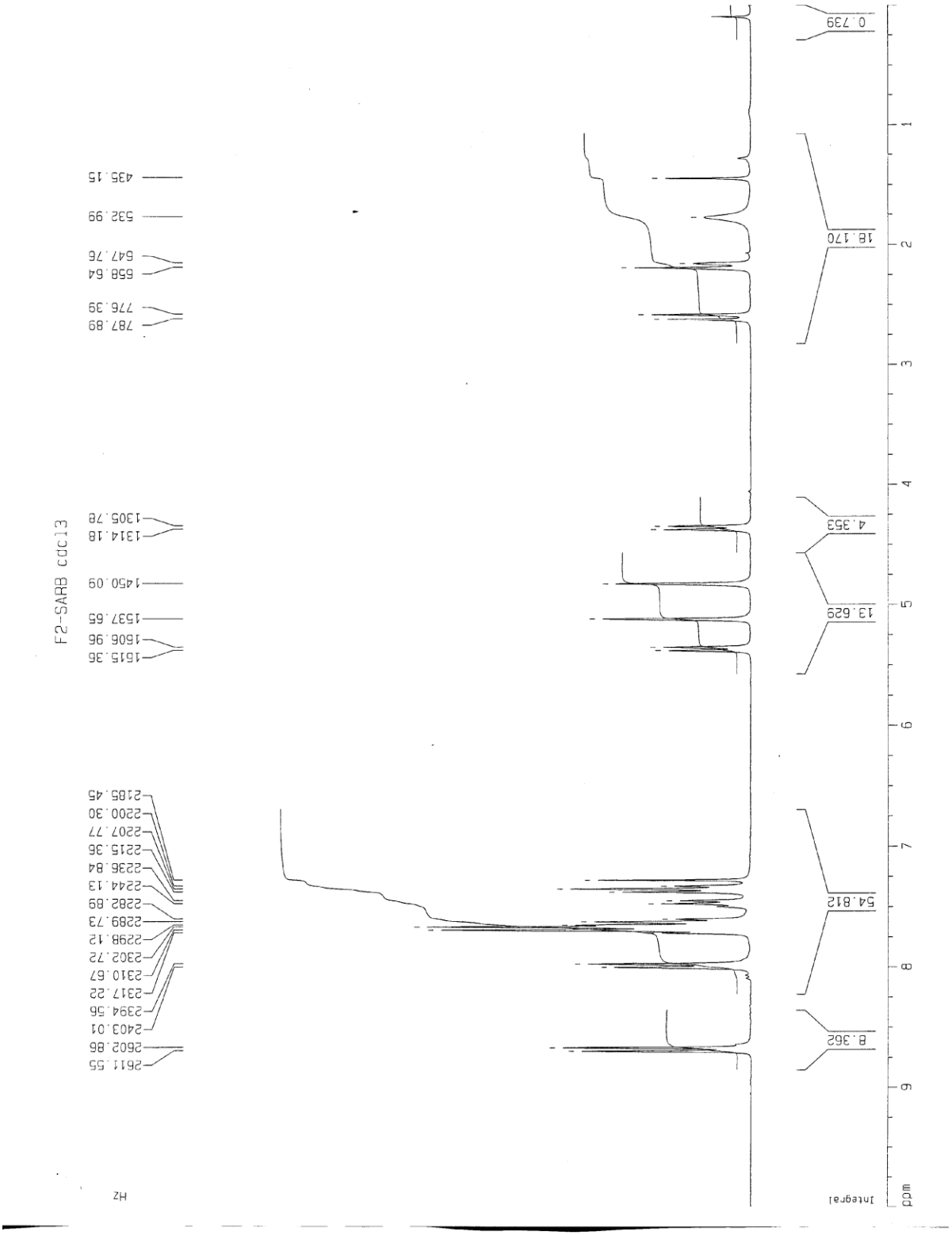
Table of Contents

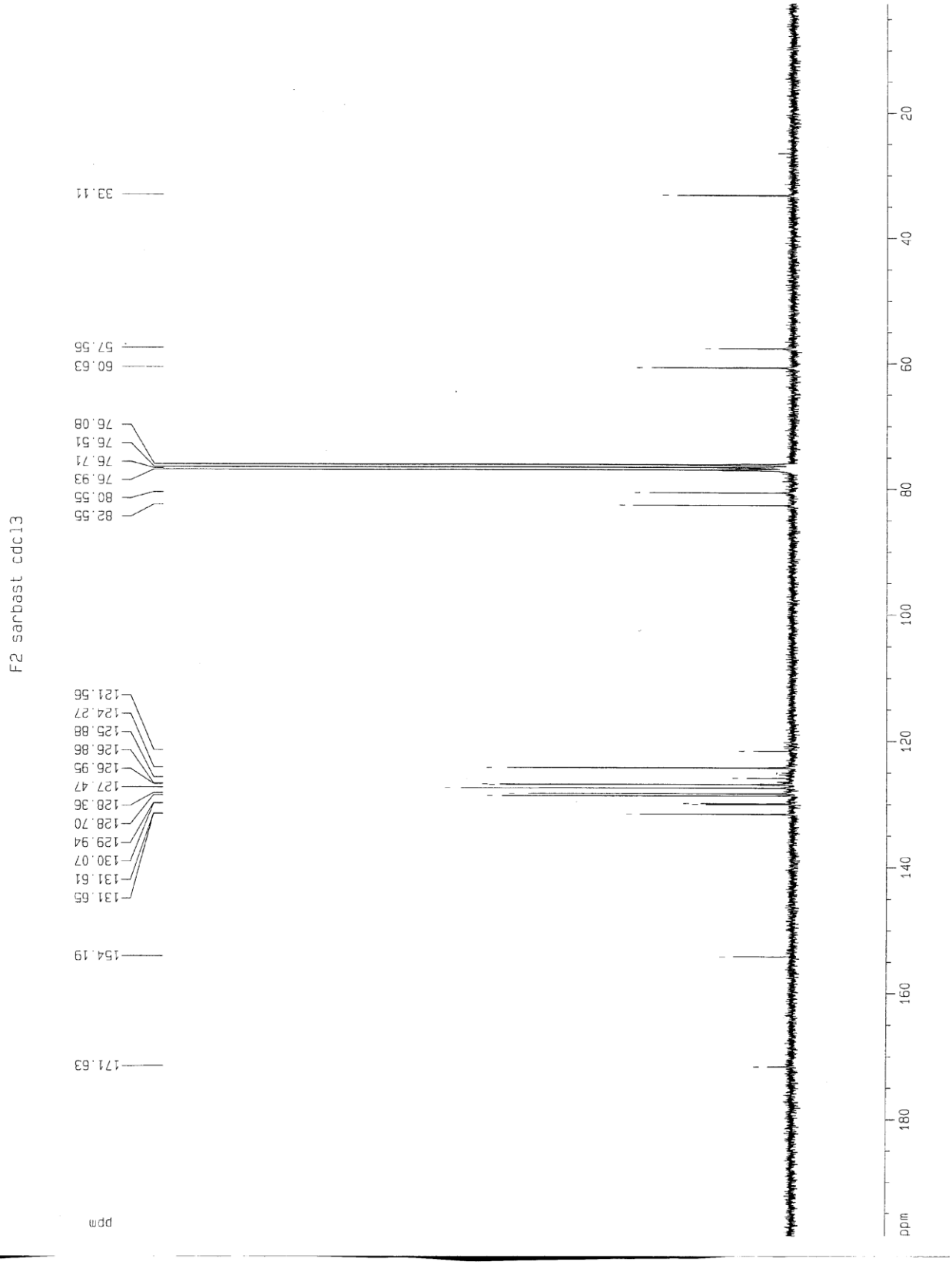
1. ^{1}H, ^{13}C and ^{31}P NMR spectra and HRMS spectra of synthetized compounds S2

2. Cartesian Coordinates of optimized structures S56

1. ^{1}H, ^{13}C and ^{31}P NMR spectra and HRMS spectra of synthetized compounds

5a

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76.08
76.51
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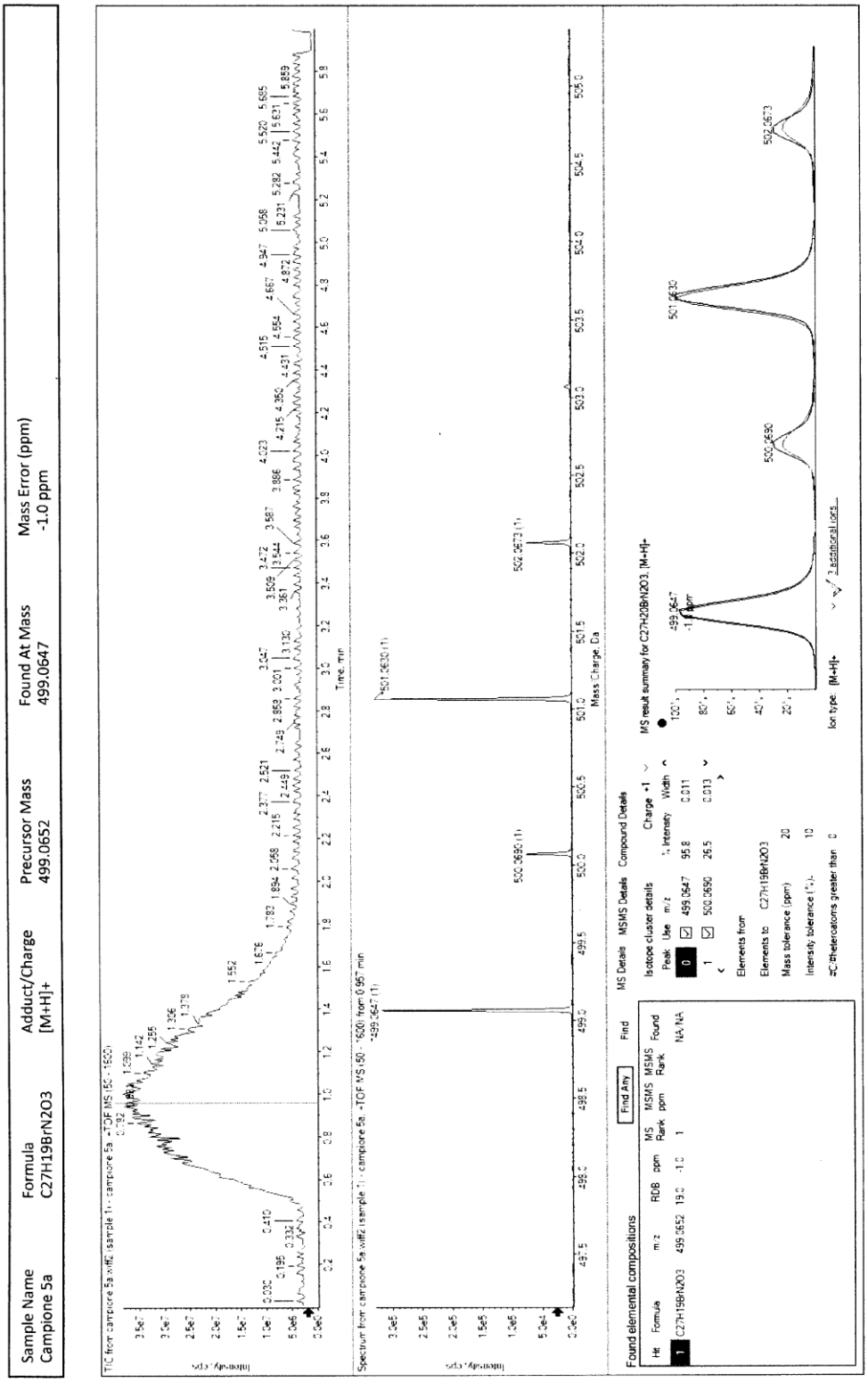
82.55
121.56
124.27
125.88
126.86
126.95
127.47
128.36
128.70
129.94
130.07
131.61
131.65
154.19
171.63
ppm
20
40
60
80
100
120
140
160
180
ppm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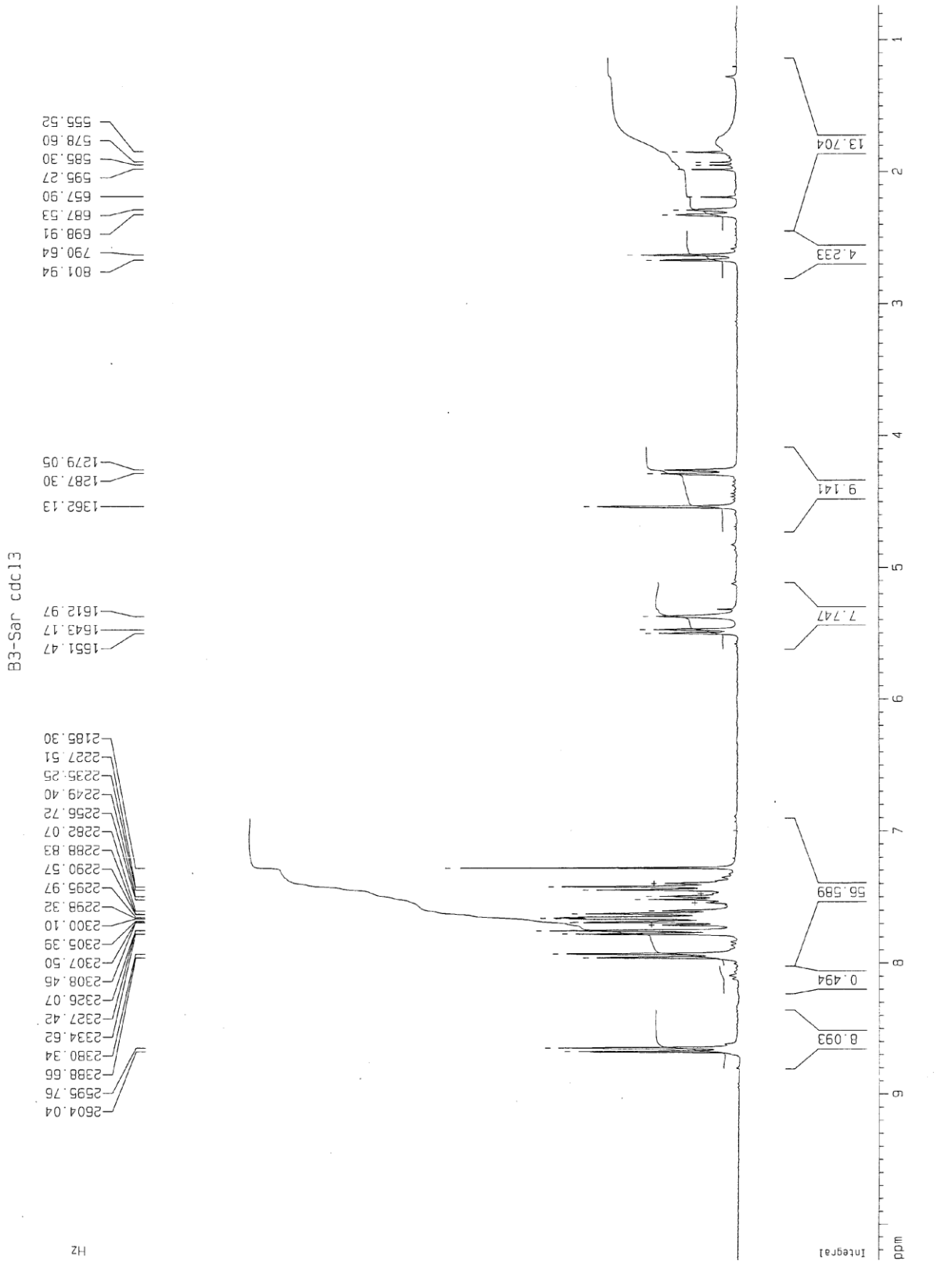
C27H19BrN2O3
Adduct/Charge
[M+H]+
Precursor Mass
499.0652
Found At Mass
499.0647
Mass Error (ppm)
-1.0 ppm
Found elemental compositions
Find Any
Find
MS Details
MSMS Details
Compound Details
Isotope cluster details
Charge +1
Peak
Use
m/z
% Intensity
Width
Elements from
Elements to C27H19BrN2O3
Mass tolerance (ppm) 20
Intensity tolerance (+/-) 10
#C-theteracatoms greater than 0
MS result summary for C27H20BrN2O3 [M+H]+
Ion type: [M+H]+
3 assignations
Time, min
Mass Charge, Da

5b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578.60
585.30
595.27
657.90
687.53
698.91
790.64
801.94
1279.05
1287.30
1362.13
1612.97
1643.17
1651.47
2185.30
2227.51
2235.25
2249.40
2256.72
2282.07
2288.83
2290.57
2295.97
2298.32
2300.10
2305.39
2307.50
2308.45
2326.07
2327.42
2334.62
2380.34
2388.66
2595.76
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H2
Integral
ppm
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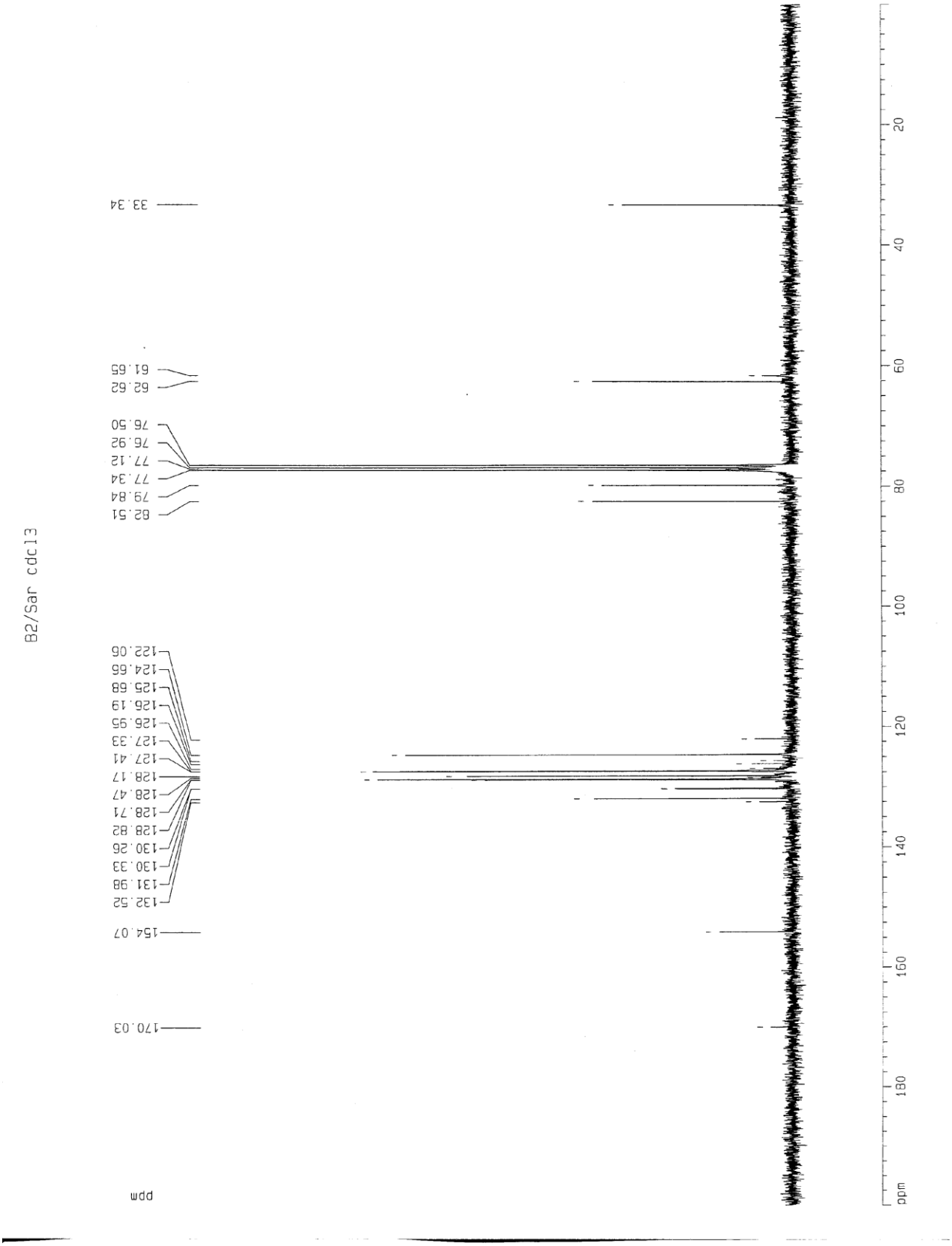
7.747
56.589
0.494
8.093


B2/Sar cdc13
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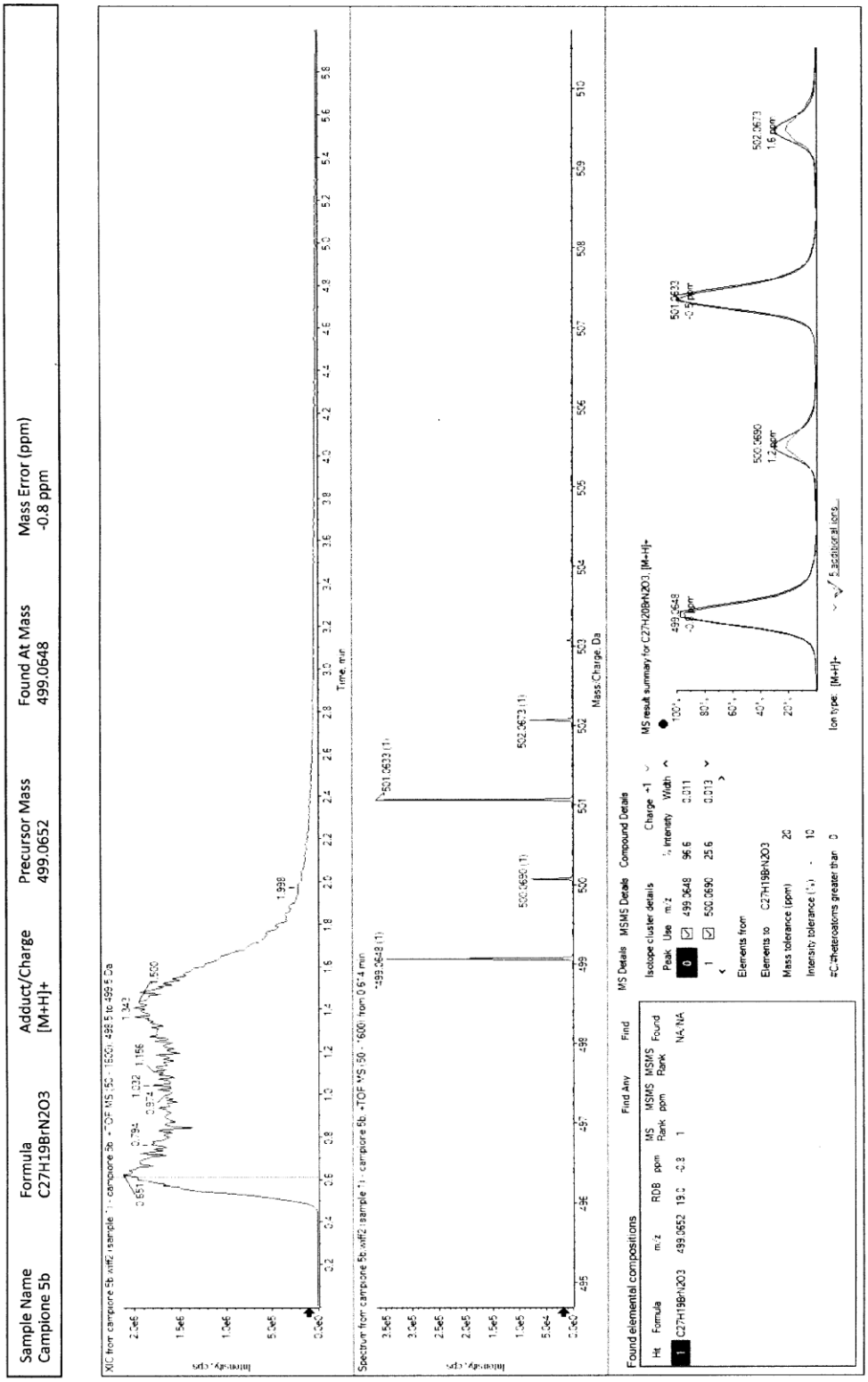
61.65
62.62
76.50
76.92
77.12
77.34
79.84
82.51
122.06
124.66
125.68
126.19
126.95
127.33
127.41
128.17
128.47
128.71
128.82
130.26
130.33
131.98
132.52
154.07
170.03
ppm
20
40
60
80
100
120
140
160
180
ppm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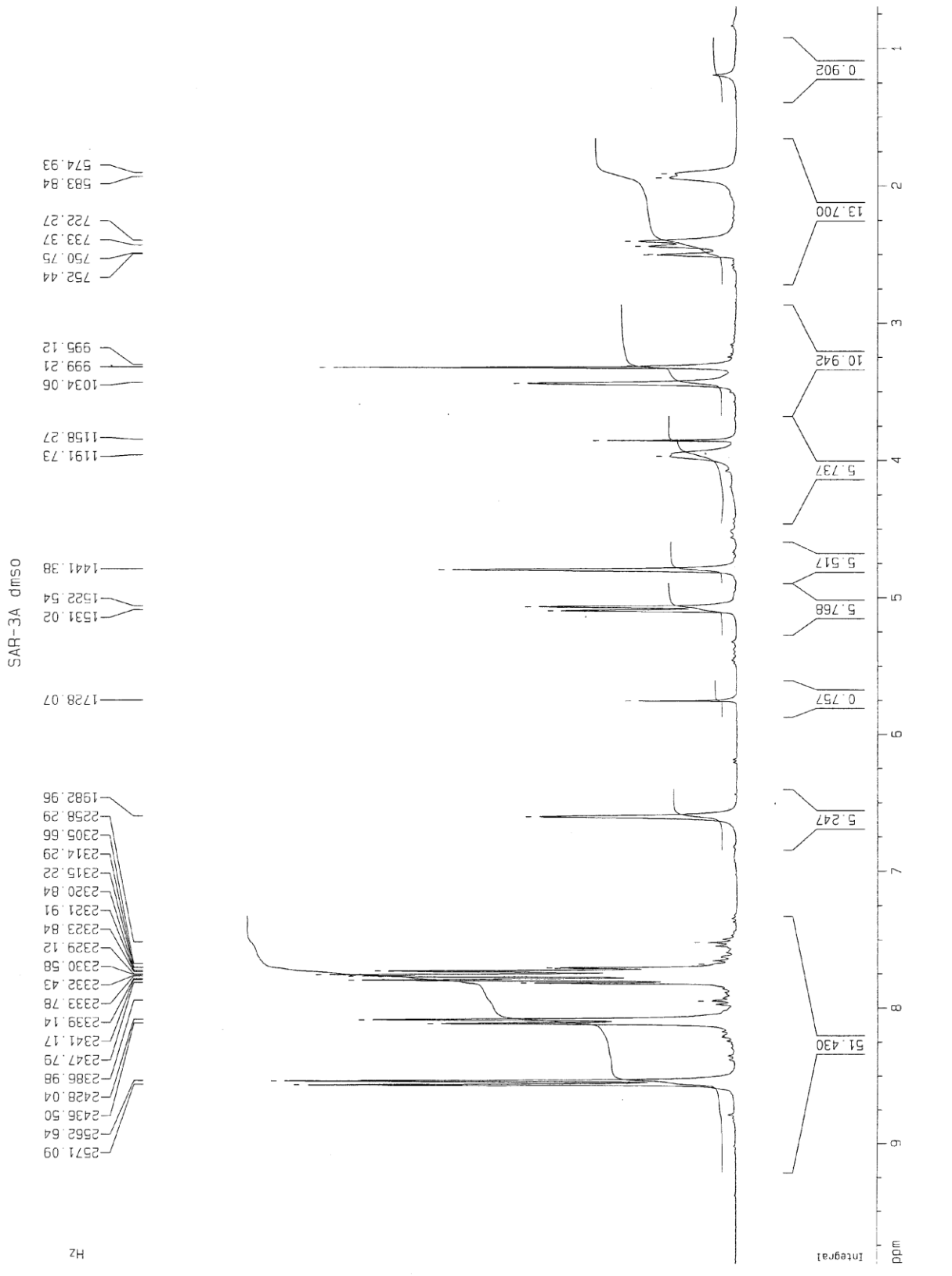
Campione 5b
Formula
C27H19BrN2O3
Adduct/Charge
[M+H]+
Precursor Mass
499.0652
Found At Mass
499.0648
Mass Error (ppm)
-0.8 ppm
Time, min
Mass/Charge, Da
Found elemental compositions
Compound Details
MS result summary for C27H20BrN2O3 [M+H]+
Ion type: [M+H]+
Additional ions

8a


SAR-3A dmso
Hz
ppm
Integral
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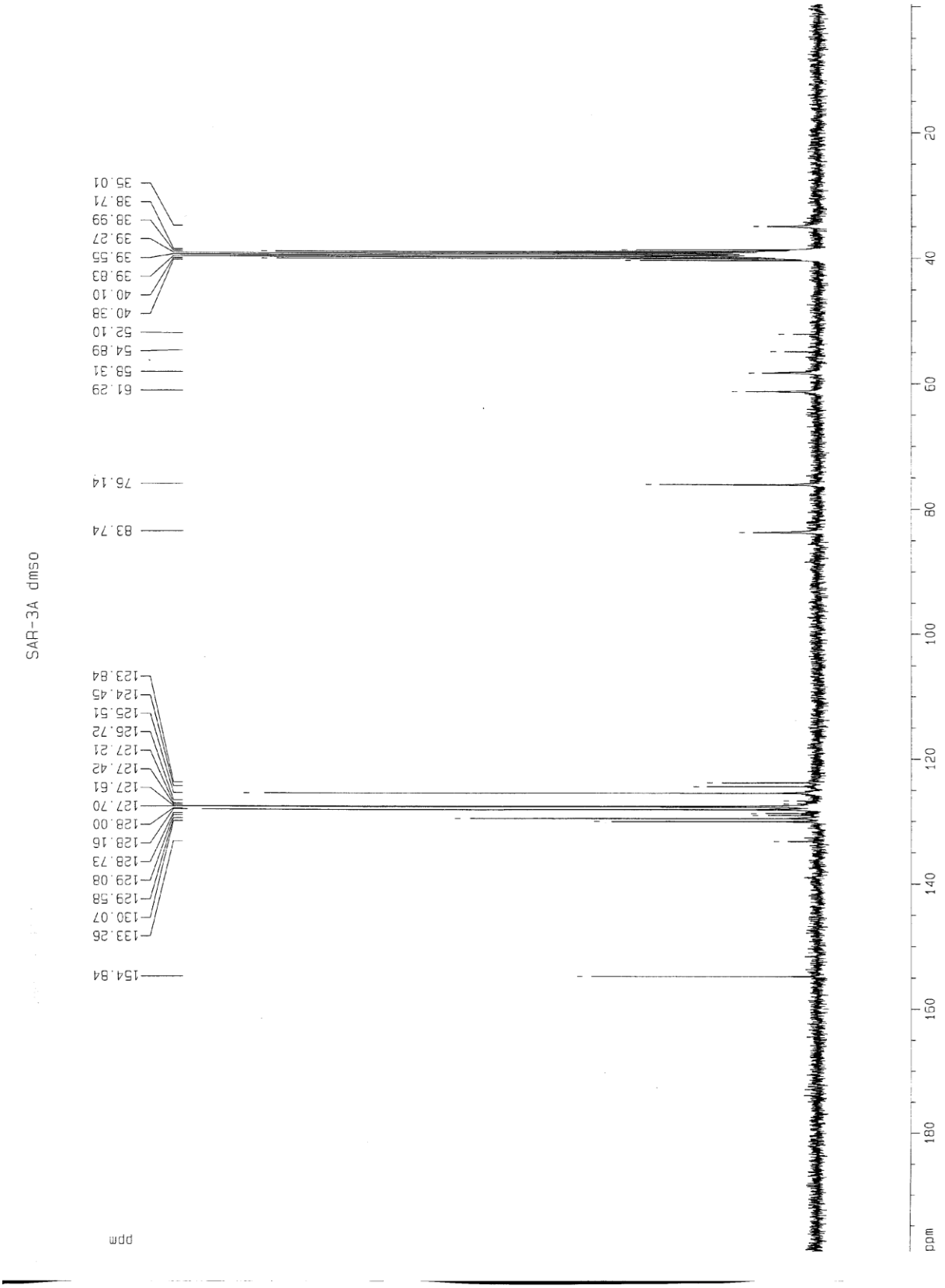
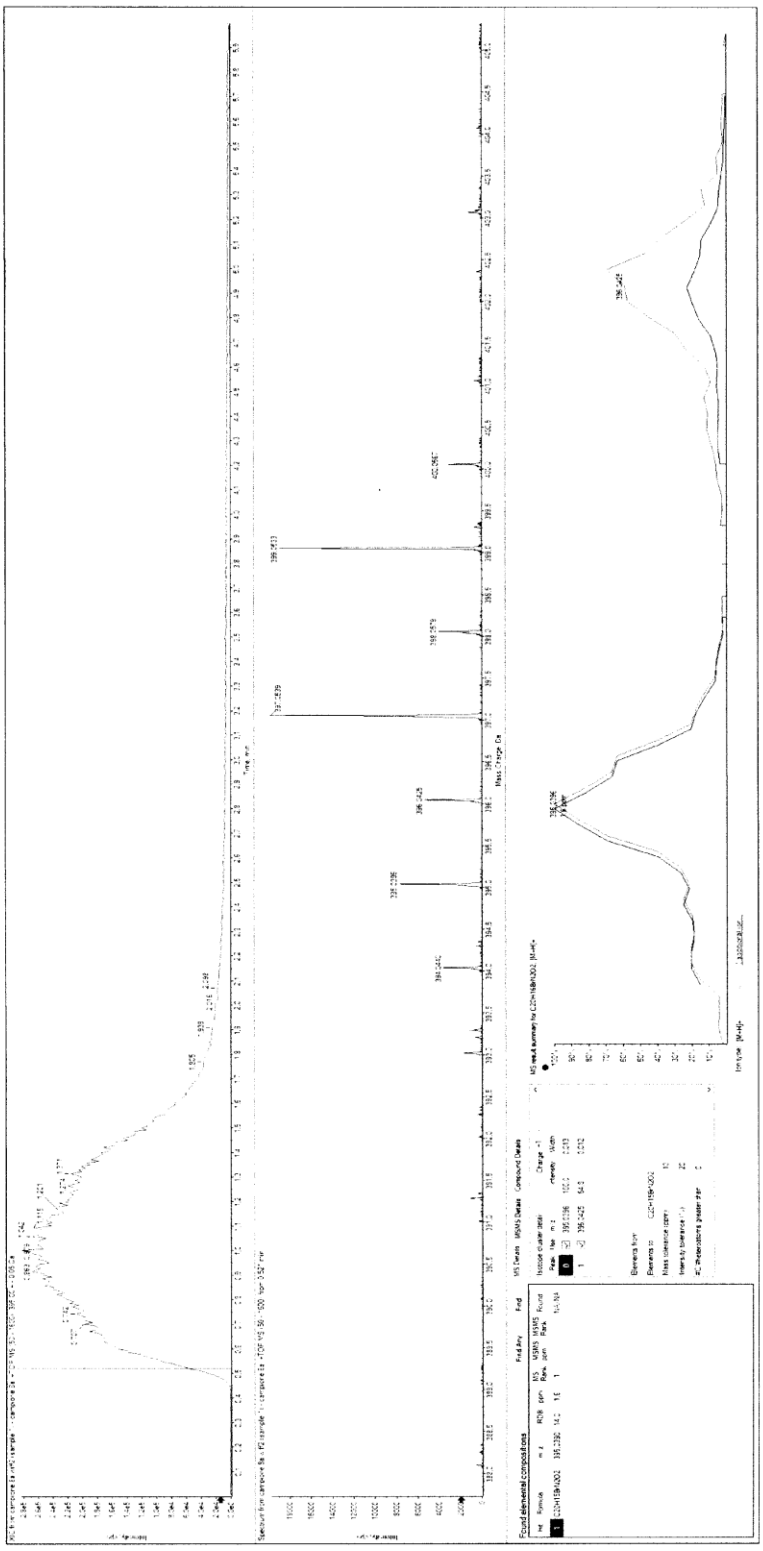
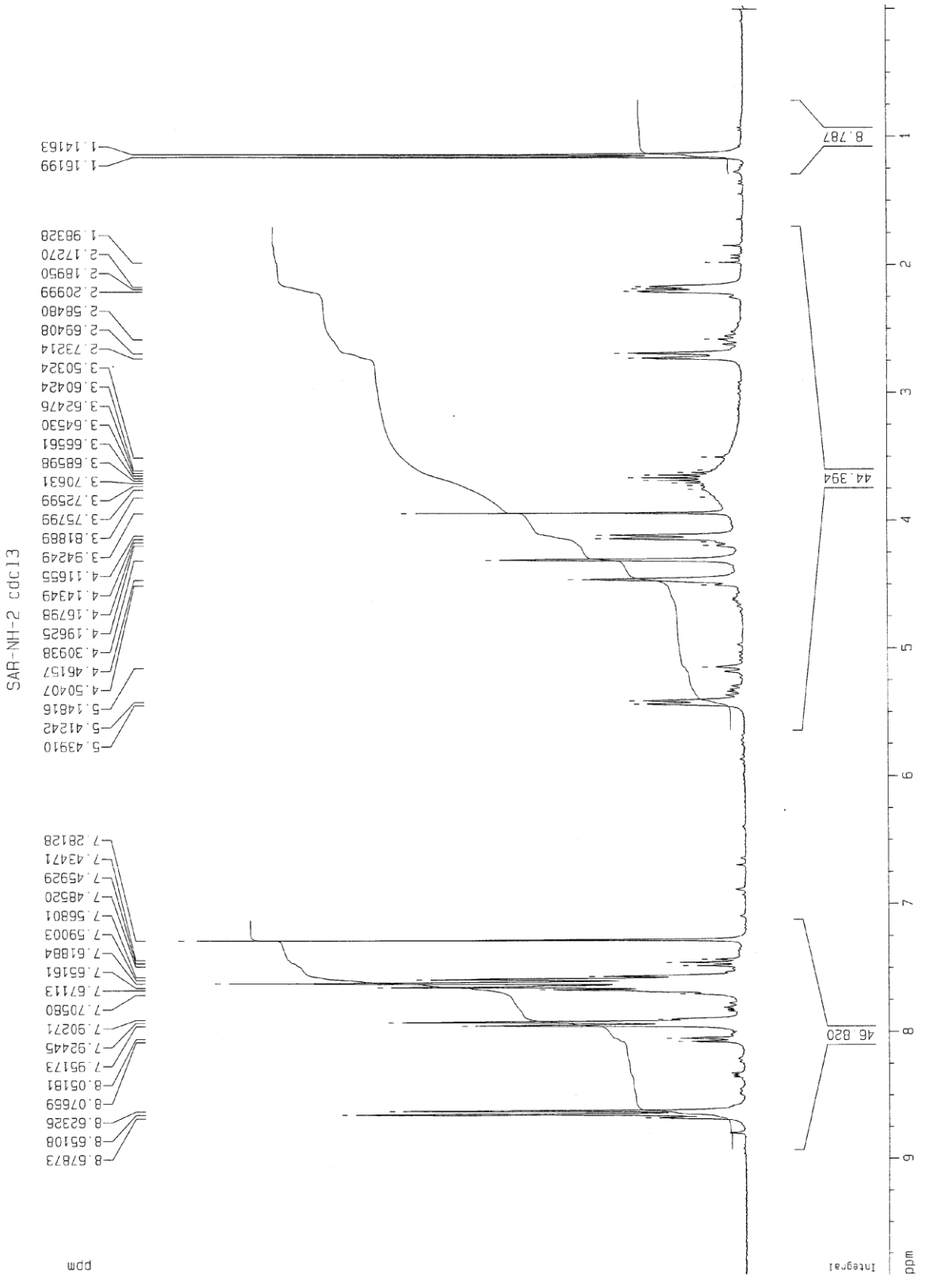
722.27
733.37
750.75
752.44
995.12
999.21
1034.06
1158.27
1191.73
1441.38
1522.54
1531.02
1728.07
1982.96
2258.29
2305.66
2314.29
2315.22
2320.84
2321.91
2323.84
2329.12
2330.58
2332.43
2333.78
2339.14
2341.17
2347.79
2386.98
2428.04
2436.50
2562.64
2571.09
0.902
13.700
10.942
5.737
5.517
5.768
0.757
5.247
51.430


SAR-3A dmso
35.01
38.71
38.99
39.27
39.55
39.83
40.10
40.38
52.10
54.89
58.31
61.29
75.14
83.74
123.84
124.45
125.51
126.72
127.21
127.42
127.61
127.70
128.00
128.15
128.73
129.08
129.58
130.07
133.26
154.84
ppm
20
40
60
80
100
120
140
150
180
ppm

Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 8a	C20H15BrN2O2	[M+H]+	395.0390	395.0396	1.6 ppm



8b


SAR-NH-2 cdcl3
1.14163
1.16199
1.98328
2.17270
2.18950
2.20999
2.58480
2.69408
2.73214
3.50324
3.60424
3.62476
3.64530
3.65561
3.68598
3.70631
3.72599
3.75799
3.81889
3.94249
4.11655
4.14349
4.16798
4.19625
4.30938
4.46157
4.50407
5.14816
5.41242
5.43910
7.28128
7.43471
7.45929
7.48520
7.56801
7.59003
7.61884
7.65161
7.67113
7.70580
7.90271
7.92445
7.95173
8.05181
8.07659
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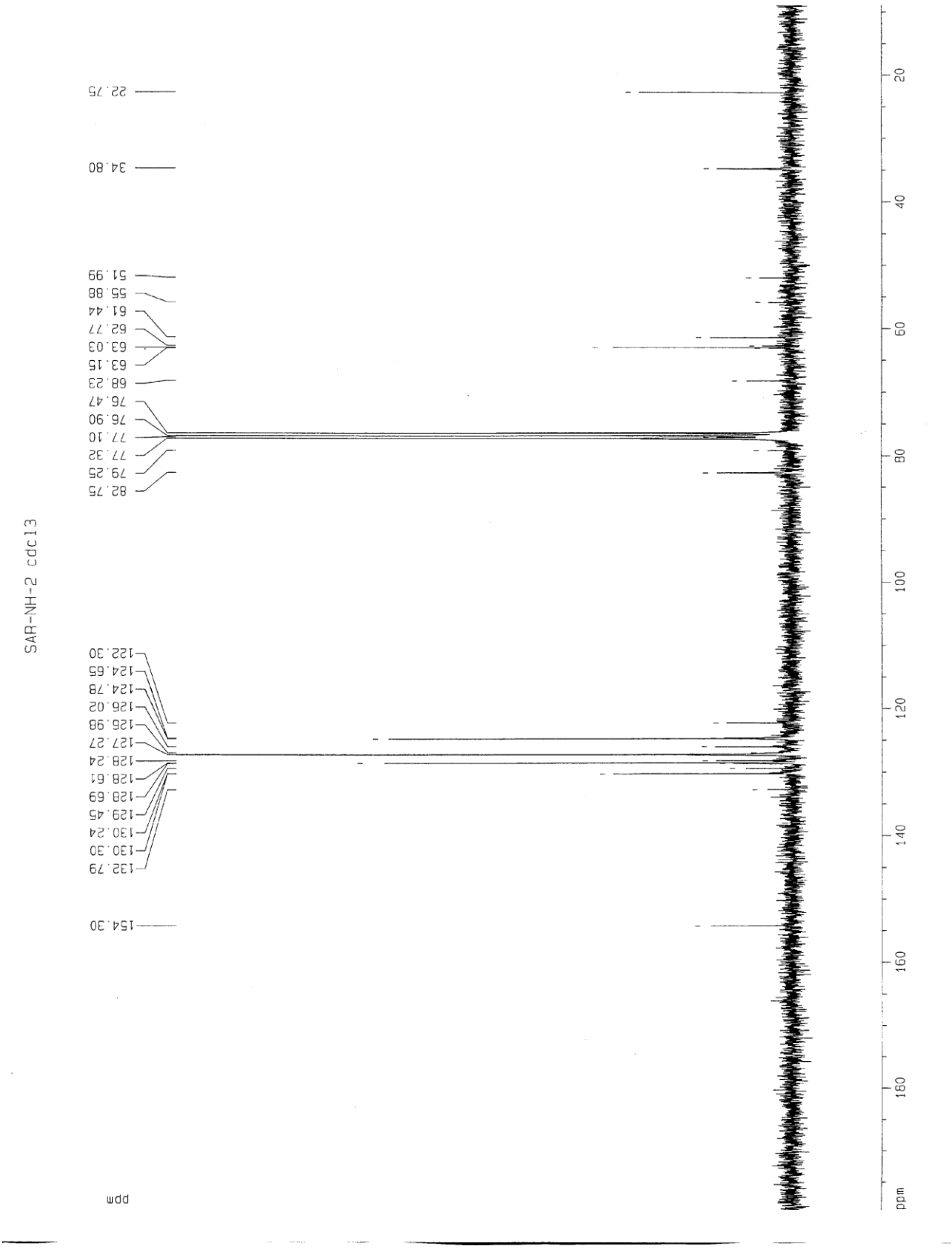
8.65108
8.67873
8.787
44.394
46.820
ppm
Integral


SAR-NH-2 cdc13
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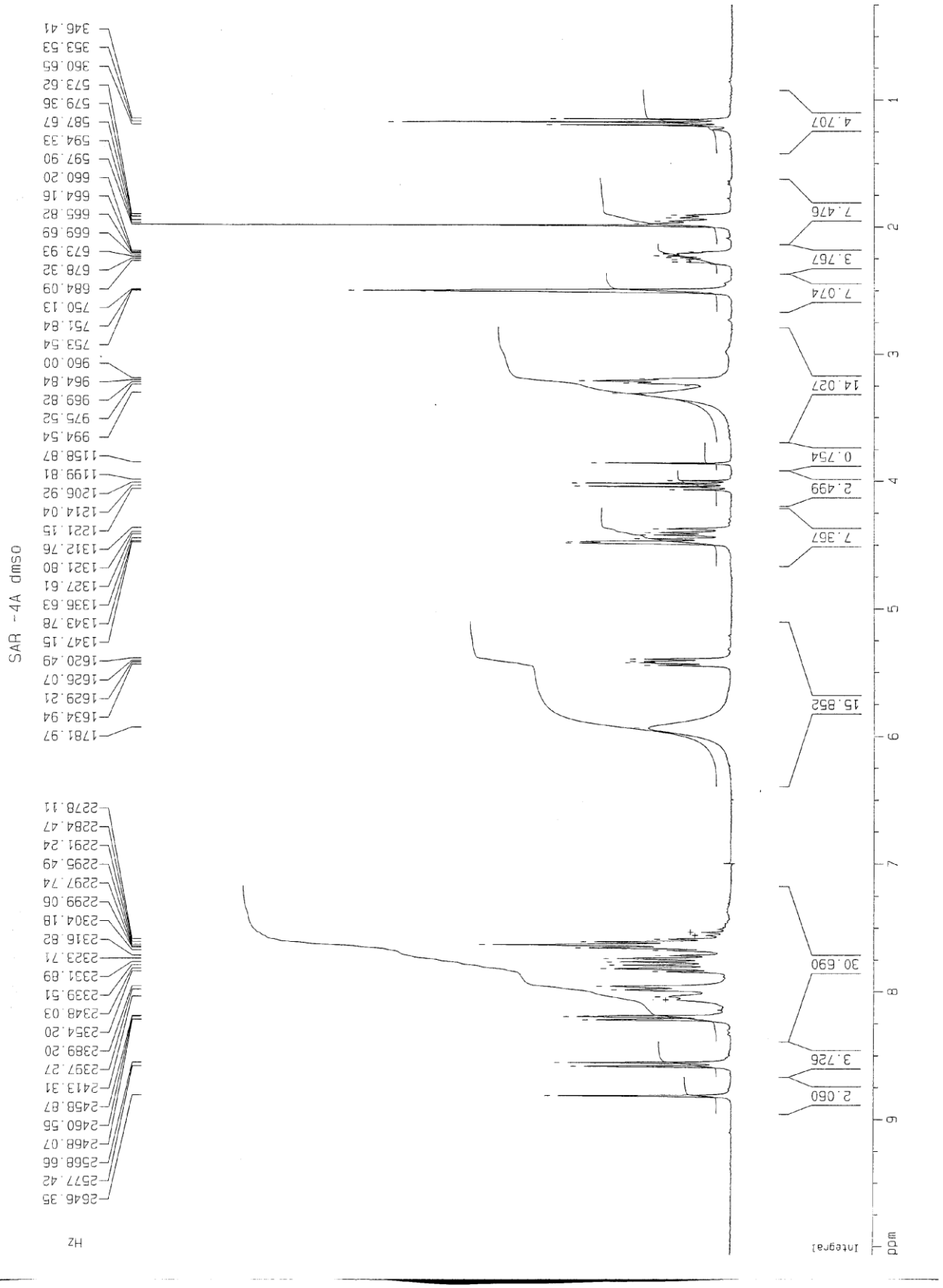
34.80
51.99
55.88
61.44
62.77
63.03
63.15
68.23
76.47
76.90
77.10
77.32
79.25
82.75
122.30
124.65
124.78
126.02
126.98
127.27
128.24
128.61
128.69
129.45
130.24
130.30
132.79
154.30
ppm
20
40
60
80
100
120
140
160
180
ppm

Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 8b	C20H15BrN2O2	[M+H]+	395.0390	395.0392	0.6 ppm

9a


SAR -4A dmso
Hz
Integral
ppm
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353.53
360.65
573.62
579.36
587.67
594.33
597.90
660.20
664.16
665.82
669.69
673.93
678.32
684.09
750.13
751.84
753.54
960.00
964.84
969.82
975.52
994.54
1158.87
1199.81
1206.92
1214.04
1221.15
1312.76
1321.80
1327.61
1336.63
1343.78
1347.15
1620.49
1626.07
1629.21
1634.94
1781.97
2278.11
2284.47
2291.24
2295.49
2297.74
2299.06
2304.18
2316.82
2323.71
2331.89
2339.51
2348.03
2354.20
2389.20
2397.27
2413.31
2458.87
2460.56
2468.07
2568.66
2577.42
2646.35
4.707
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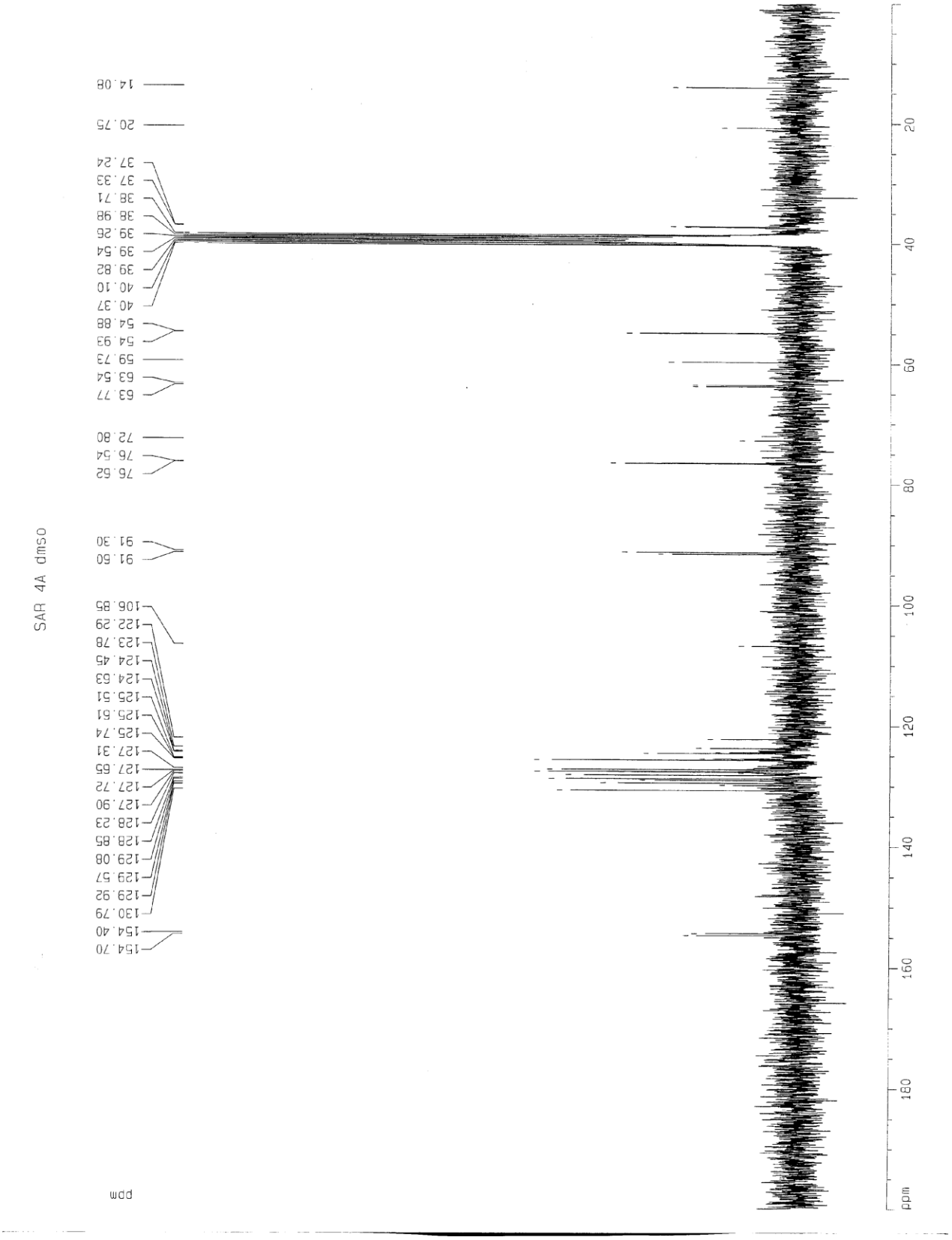
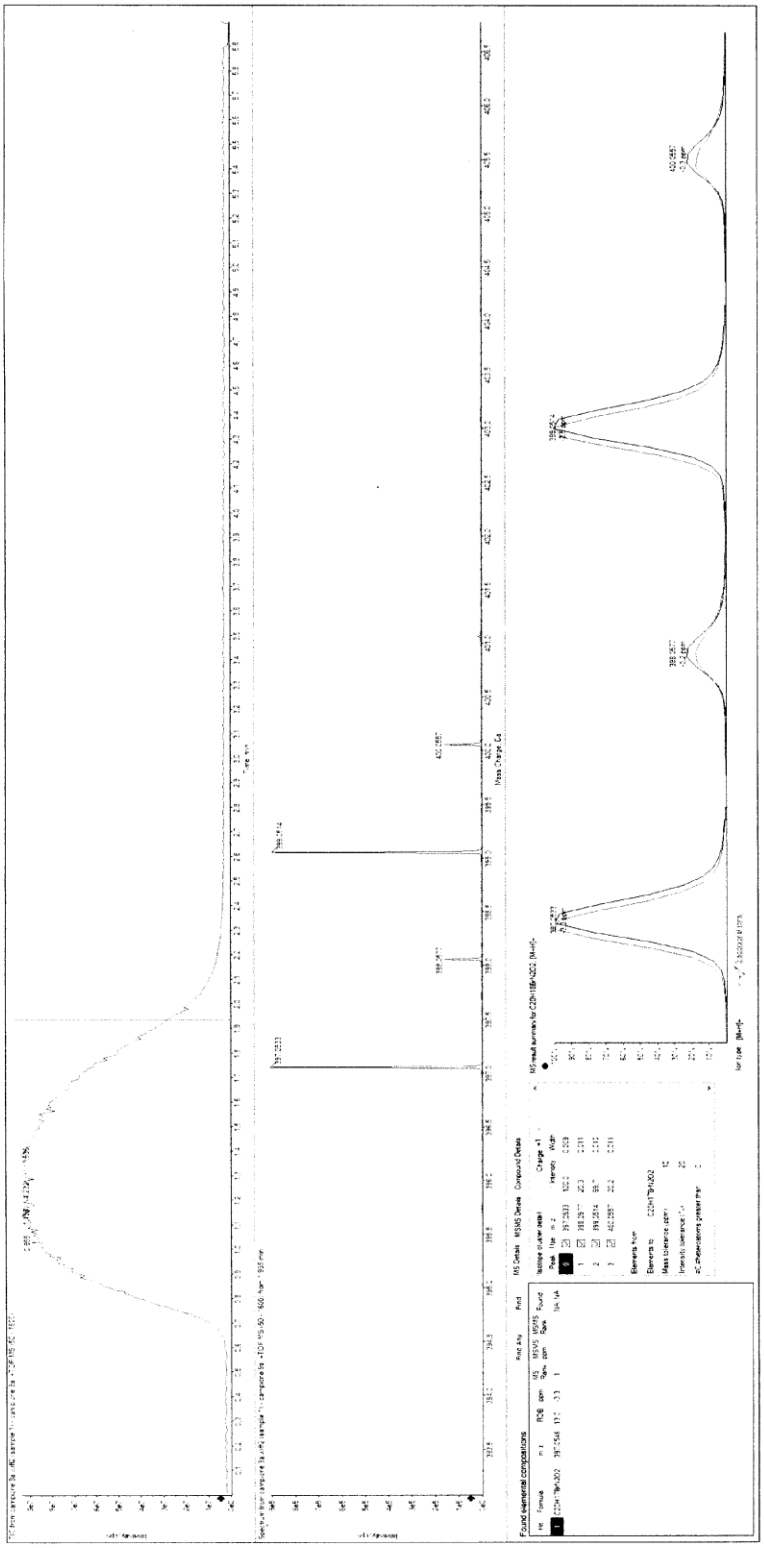
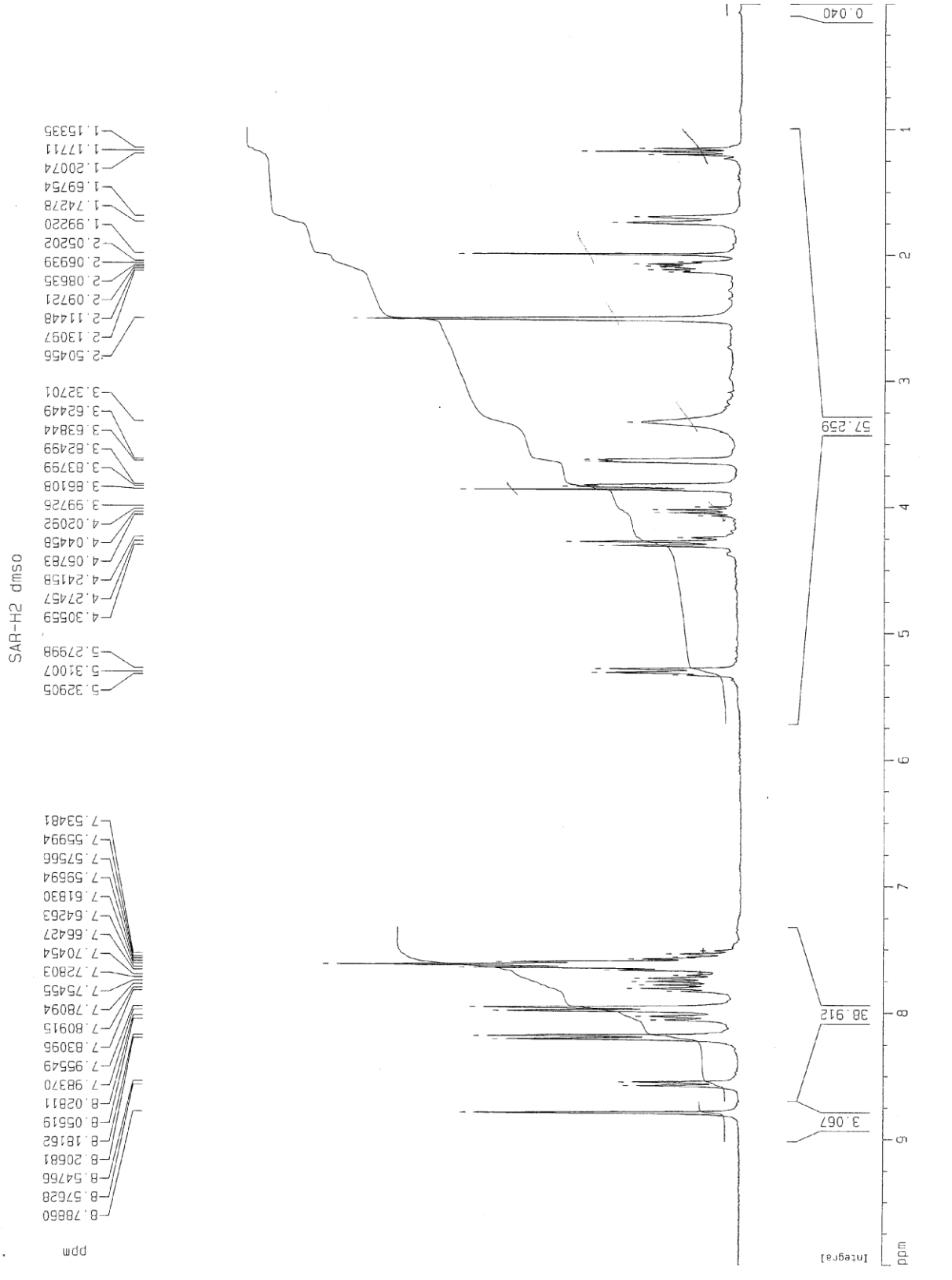
3.767
7.074
14.027
0.754
2.499
7.367
15.852
30.690
3.726
2.060


SAR 4A dmso
14.08
20.75
37.24
37.33
38.71
38.98
39.26
39.54
39.82
40.10
40.37
54.88
54.93
59.73
63.54
63.77
72.80
76.54
76.62
91.30
91.60
106.85
122.29
123.78
124.45
124.63
125.51
125.61
125.74
127.31
127.65
127.72
127.90
128.23
128.85
129.08
129.57
129.92
130.79
154.40
154.70
ppm
20
40
60
80
100
120
140
160
180
ppm

Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 9a	C20H17BrN2O2	[M+H]+	397.0546	397.0533	-3.3 ppm



9b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1.17711
1.20074
1.69754
1.74278
1.99220
2.05202
2.06939
2.08635
2.09721
2.11448
2.13097
2.50455
3.32701
3.62449
3.63844
3.82499
3.83799
3.86108
3.99725
4.02092
4.04458
4.05783
4.24158
4.27457
4.30559
5.27998
5.31007
5.32905
7.53481
7.55994
7.57566
7.59594
7.61830
7.64263
7.66427
7.70454
7.72803
7.75455
7.78094
7.80915
7.83096
7.95549
7.98370
8.02811
8.05519
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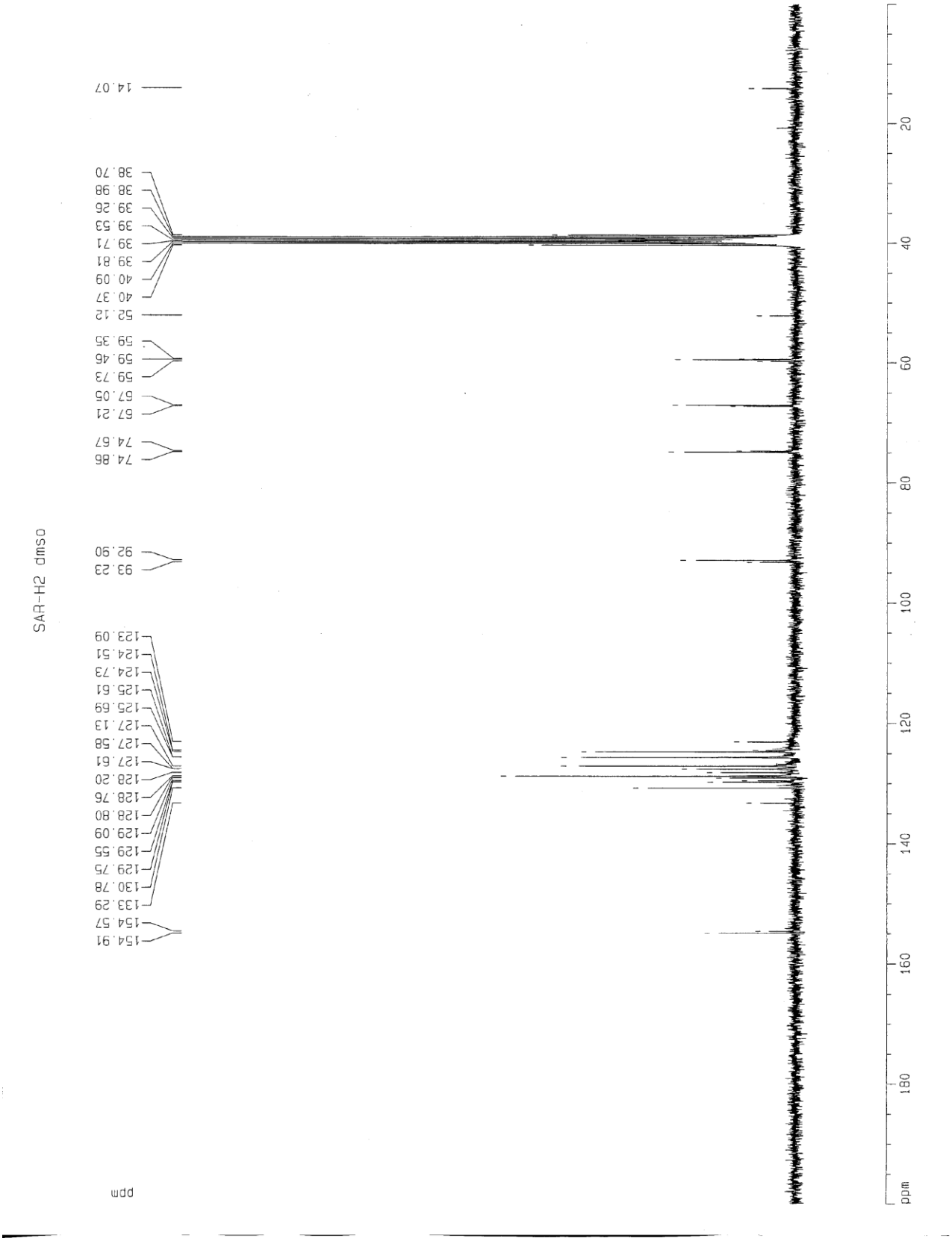
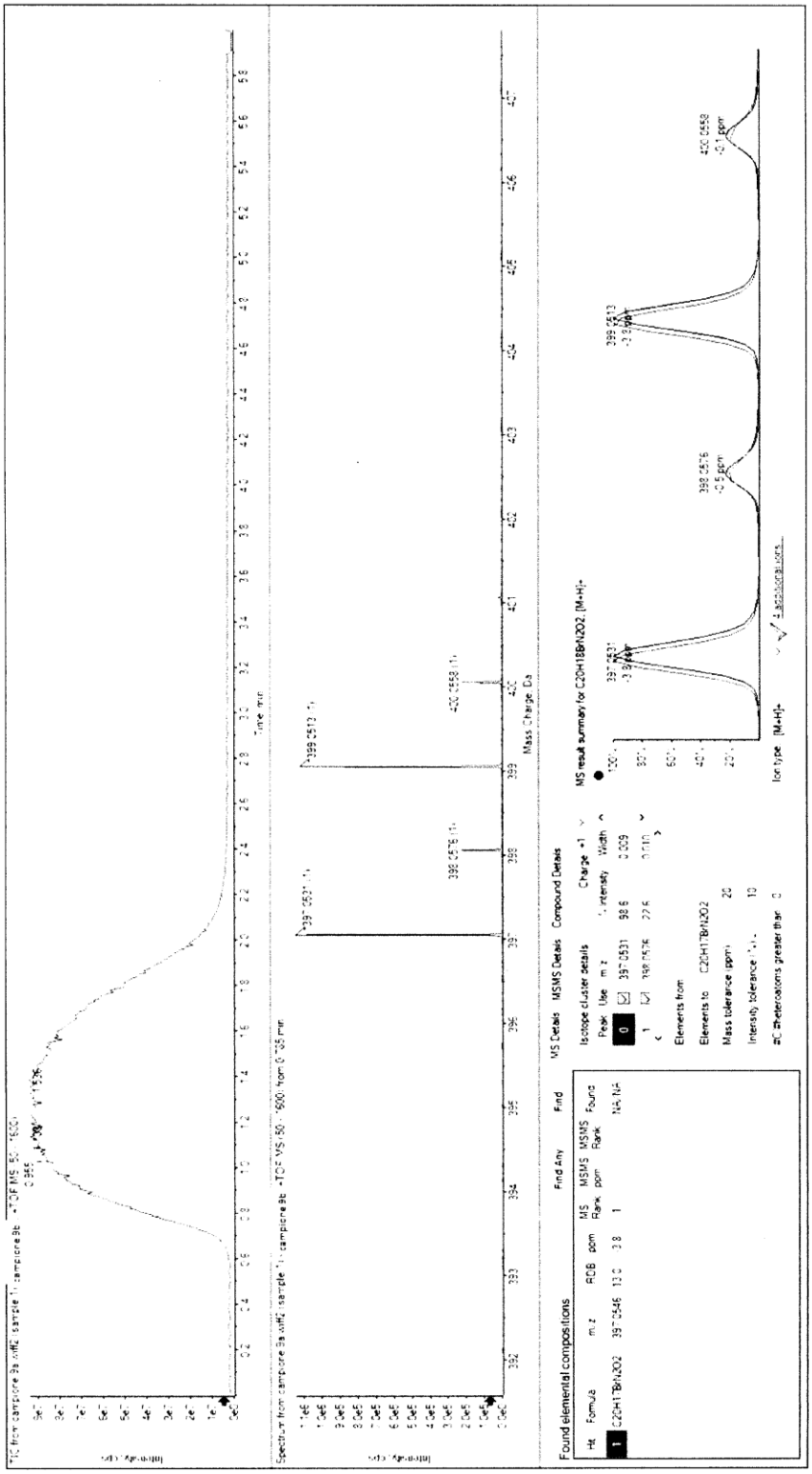
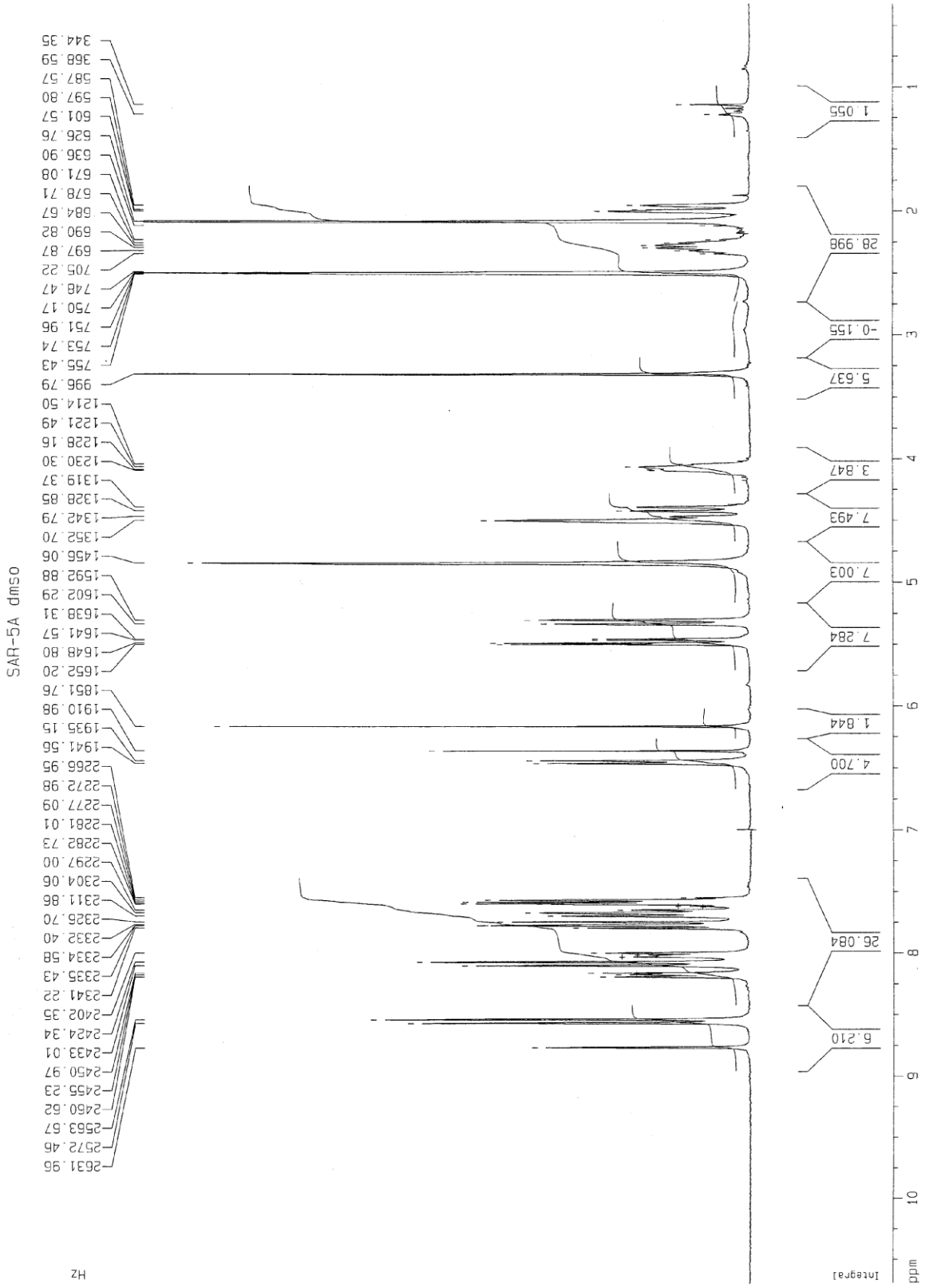
Integral
ppm


SAR-H2 dmso
14.07
38.70
38.98
39.26
39.53
39.71
39.81
40.09
40.37
52.12
59.35
59.46
59.73
67.05
67.21
74.67
74.86
92.90
93.23
123.09
124.51
124.73
125.61
125.69
127.13
127.58
127.61
128.20
128.76
128.80
129.09
129.55
129.75
130.78
133.29
154.57
154.91
ppm
20
40
60
80
100
120
140
160
180
ppm

Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 9b	C20H17BrN2O2	[M+H]+	397.0546	397.0531	-3.8 ppm



10a


SAR-5A dmso
Hz
Integral
ppm
1.055
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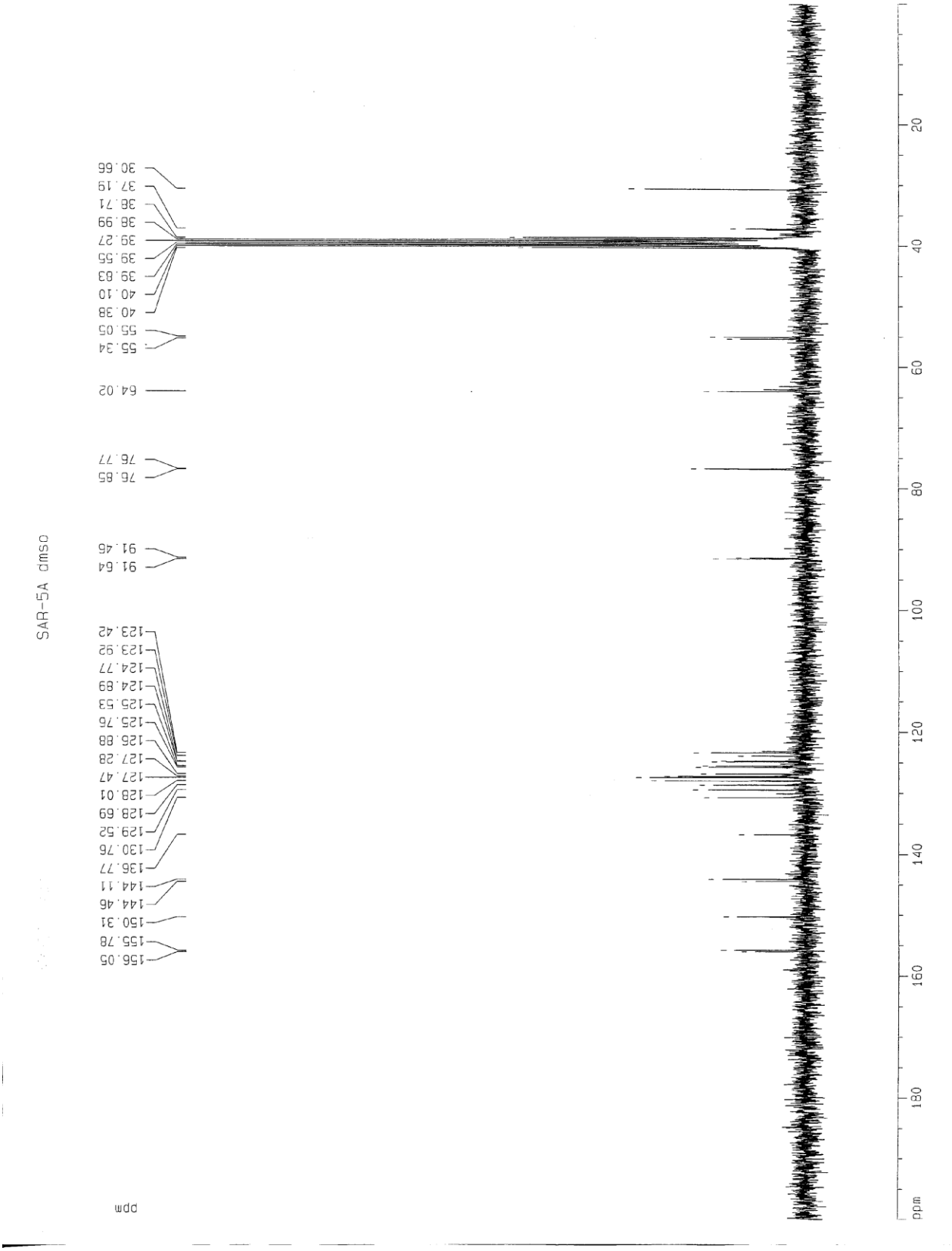
5.637
3.847
7.493
7.003
7.284
1.844
4.700
26.084
6.210


SAR-5A dmso
30.66
37.19
38.71
38.99
39.27
39.55
39.83
40.10
40.38
55.05
55.34
64.02
76.77
76.85
91.46
91.64
123.42
123.92
124.77
124.89
125.53
125.76
126.88
127.28
127.47
128.01
128.69
129.52
130.76
136.77
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150.31
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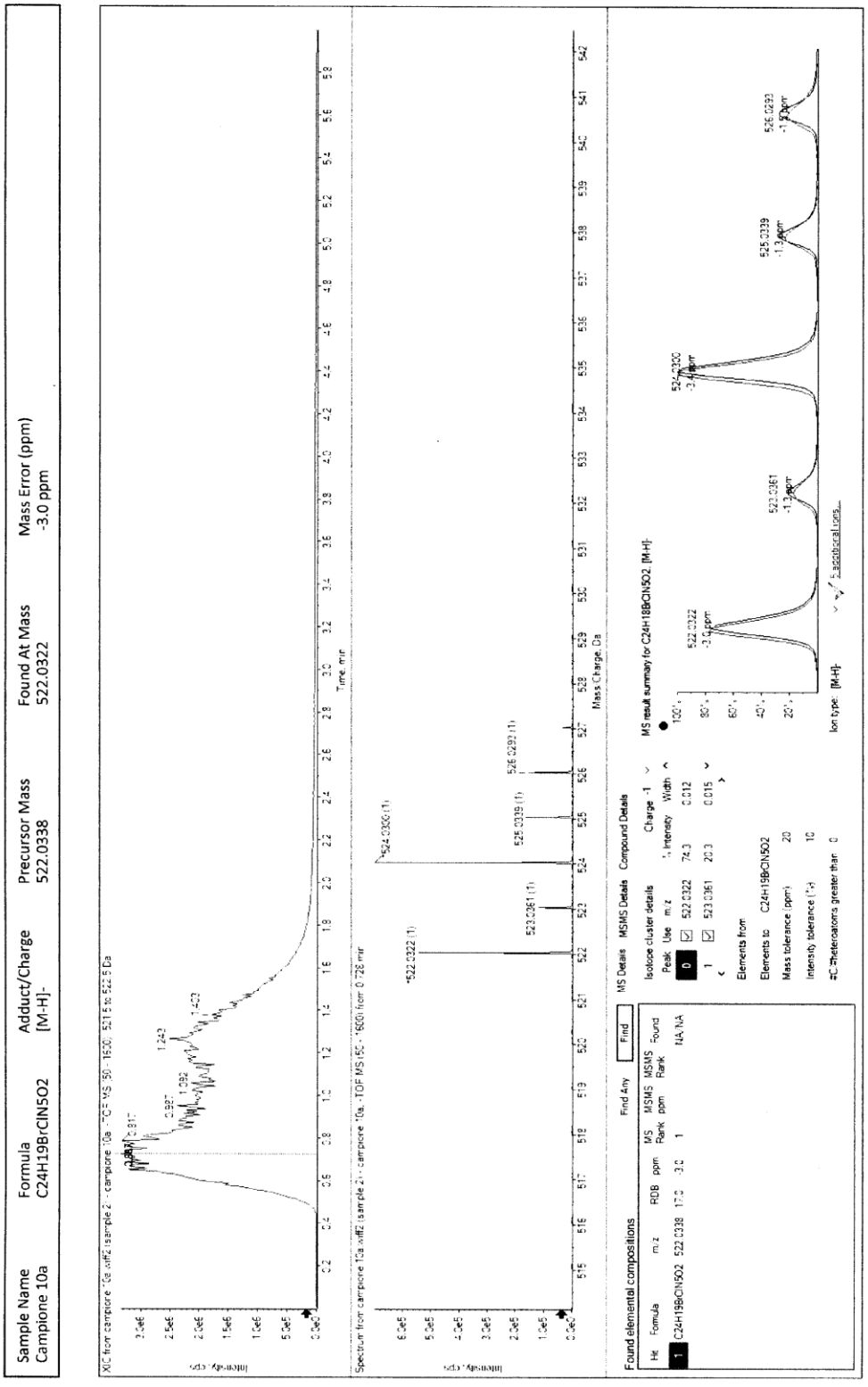
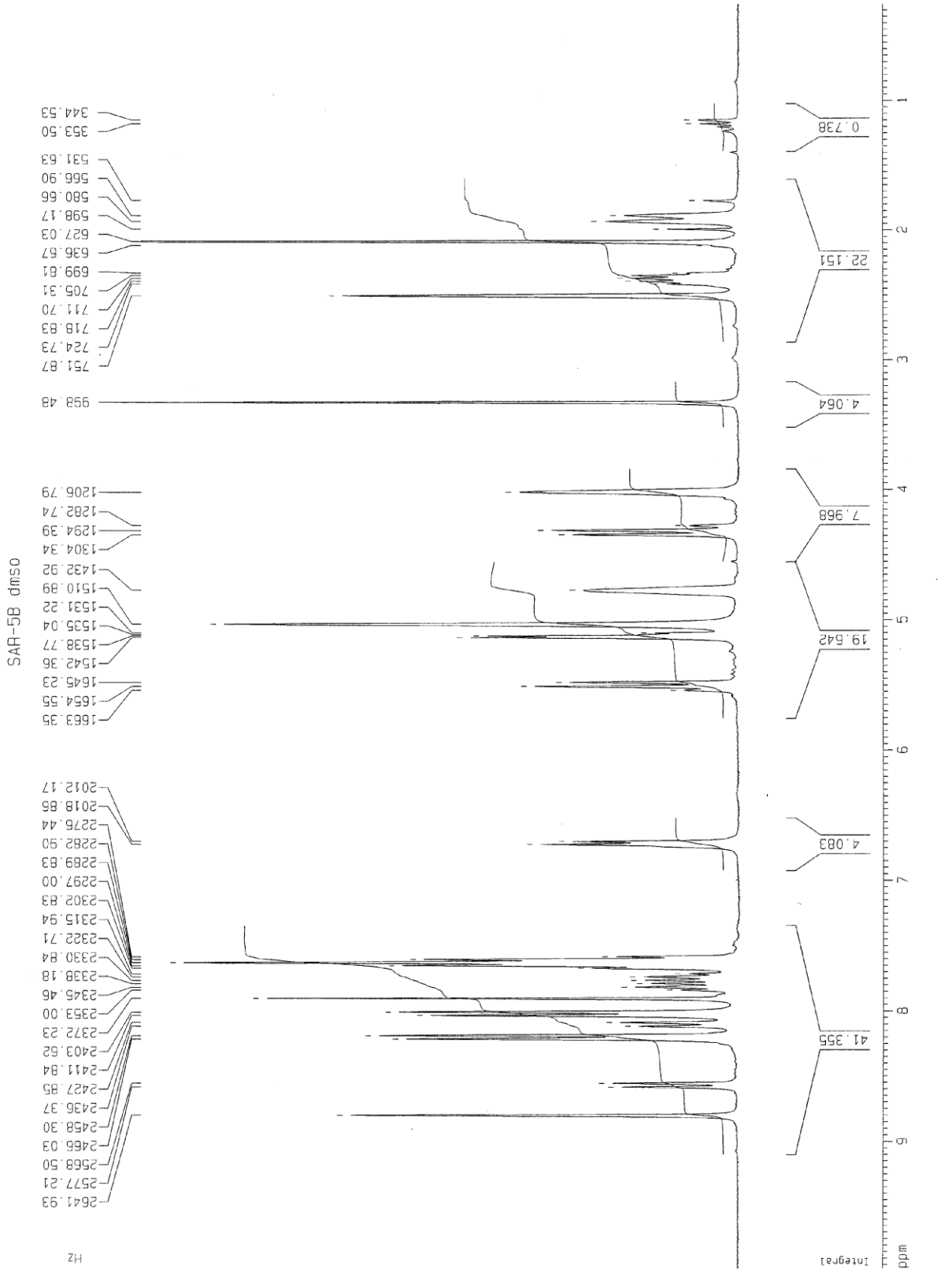
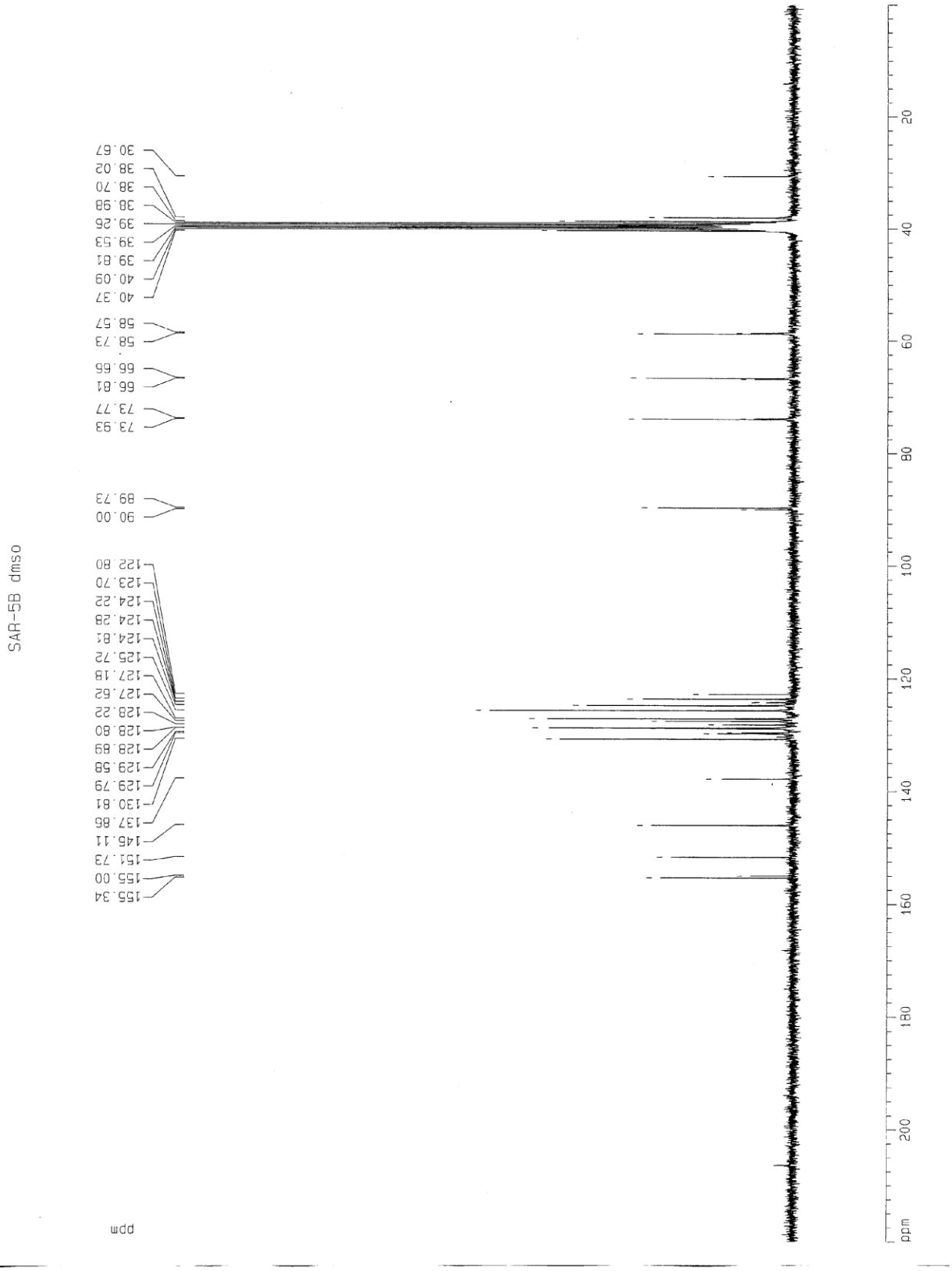
20
40
60
80
100
120
140
160
180
ppm

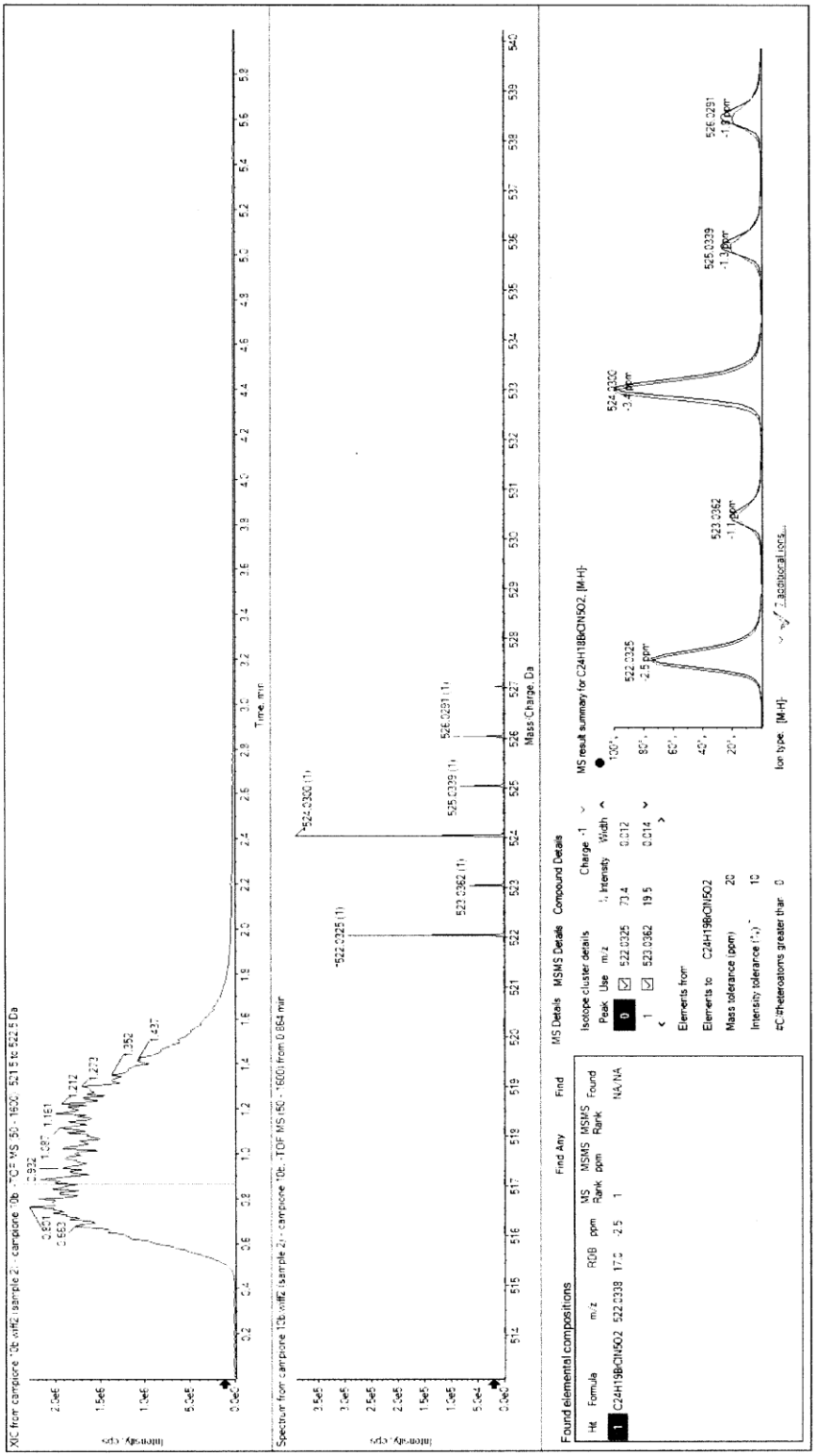

Sample Name
Campione 10a
Formula
C24H19BrCIN5O2
Adduct/Charge
[M-H]-
Precursor Mass
522.0338
Found At Mass
522.0322
Mass Error (ppm)
-3.0 ppm
Time, min
Mass Charge, Da
Found elemental compositions
MS Details
MSMS Details
Compound Details
Find
Find Any
Isotope cluster details
MS result summary for C24H18BrCIN5O2 [M-H]-
Elements from
Elements to C24H19BrCIN5O2
Mass tolerance (ppm) 20
Intensity tolerance (%) 10
#C-13heteroatoms greater than 0
Ion type: [M-H]-
Recalibrations

10b

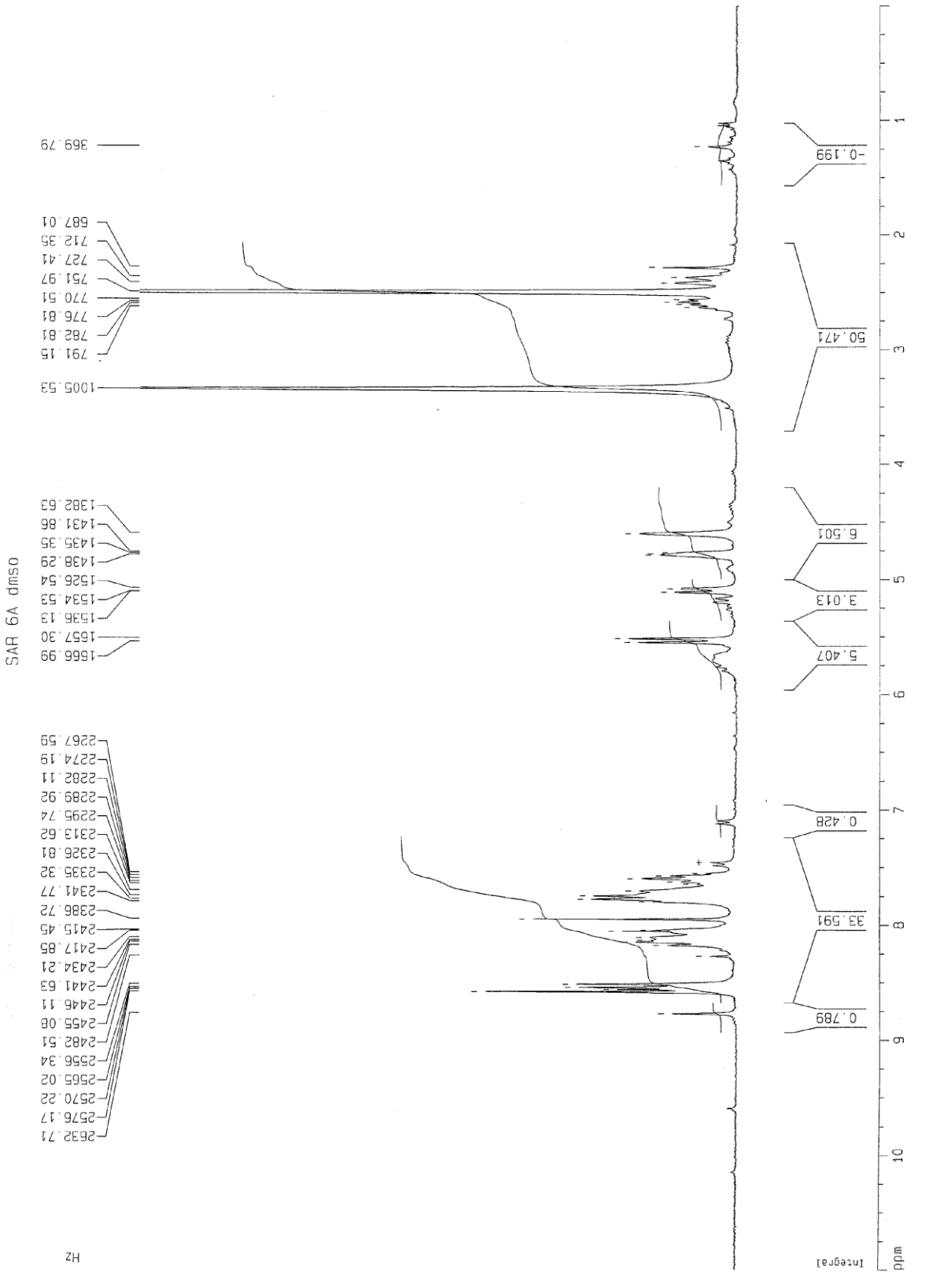

SAR-5B dmso
344.53
353.50
531.63
566.90
580.66
598.17
627.03
636.67
699.81
705.31
711.70
718.83
724.73
751.87
958.48
1206.79
1282.74
1294.39
1304.34
1432.92
1510.89
1531.22
1535.04
1538.77
1542.36
1645.23
1654.55
1663.35
2012.17
2018.85
2276.44
2282.90
2289.83
2297.00
2302.83
2315.94
2322.71
2330.84
2338.18
2345.46
2353.00
2372.23
2403.62
2411.84
2427.85
2436.37
2458.30
2466.03
2568.50
2577.21
2641.93
H2
0.738
22.151
4.064
7.968
19.542
4.083
41.355
Integral
ppm

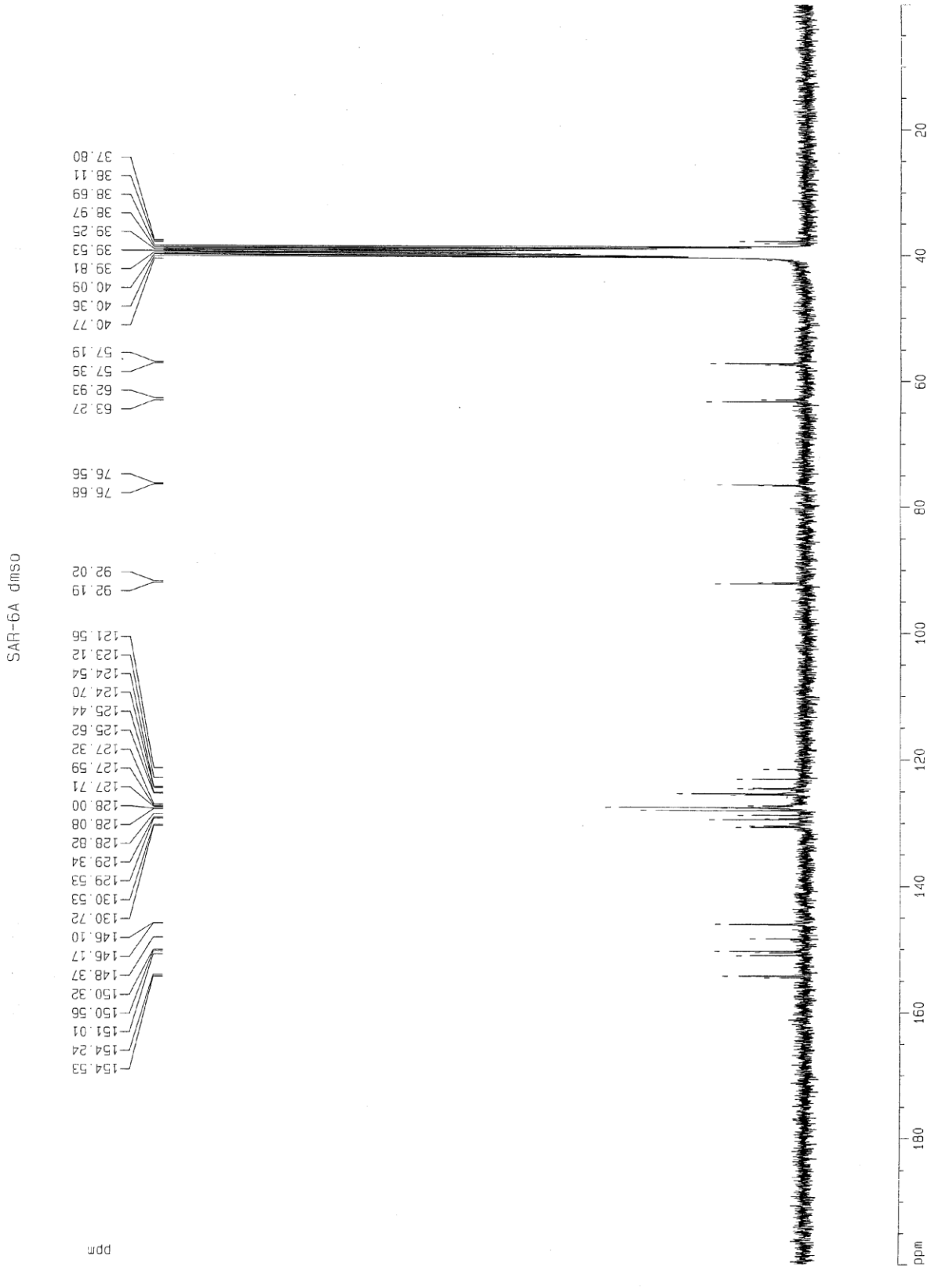

SAR-5B dmso
30.67
38.02
38.70
38.98
39.26
39.53
39.81
40.09
40.37
58.57
58.73
66.65
66.81
73.77
73.93
89.73
90.00
122.80
123.70
124.22
124.28
124.81
125.72
127.18
127.62
128.22
128.80
128.89
129.58
129.79
130.81
137.86
146.11
151.73
155.00
155.34
ppm
20
40
60
80
100
120
140
160
180
200
ppm

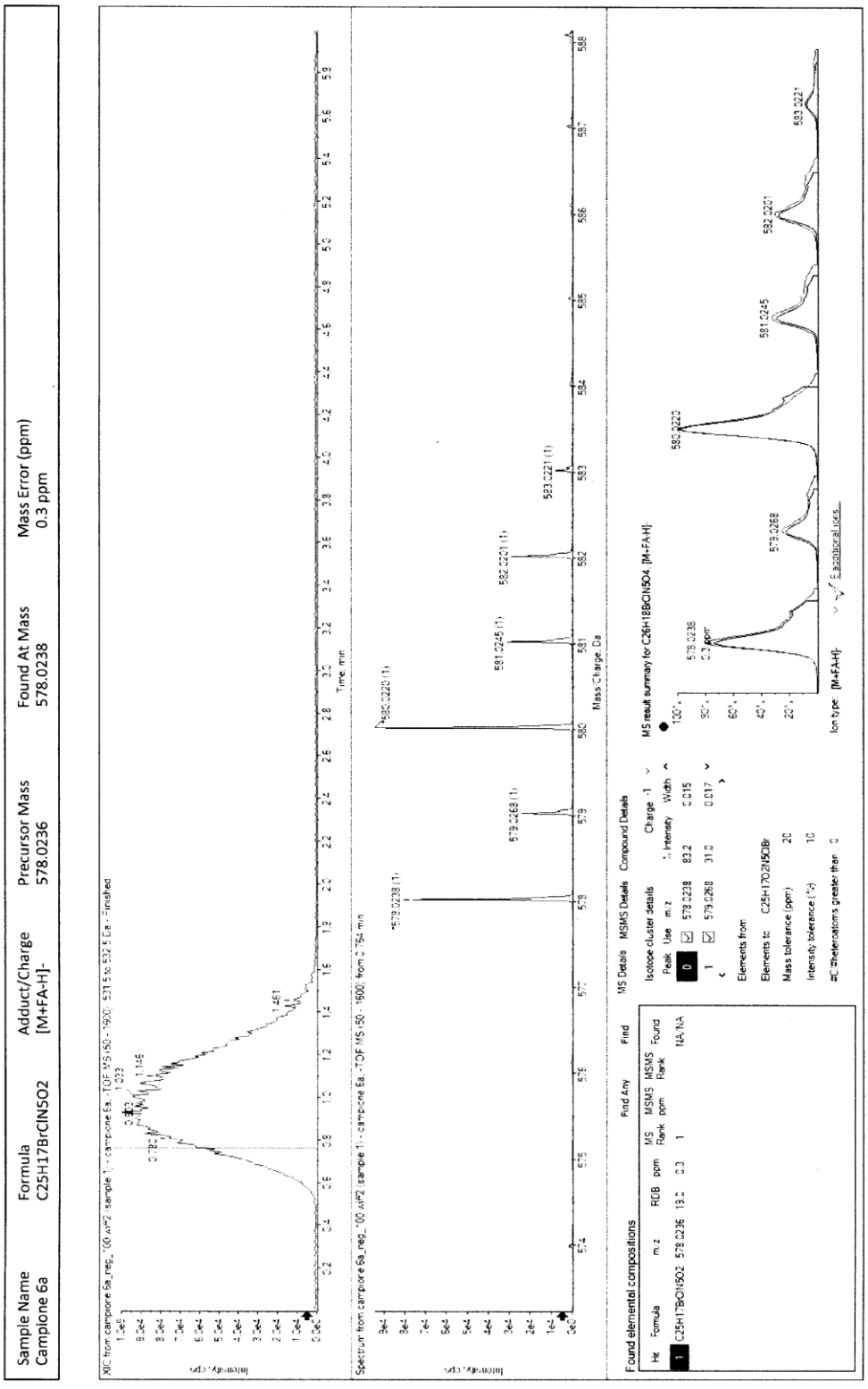
Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 10b	C24H19BrClN5O2	[M-H]-	522.0338	522.0325	-2.5 ppm



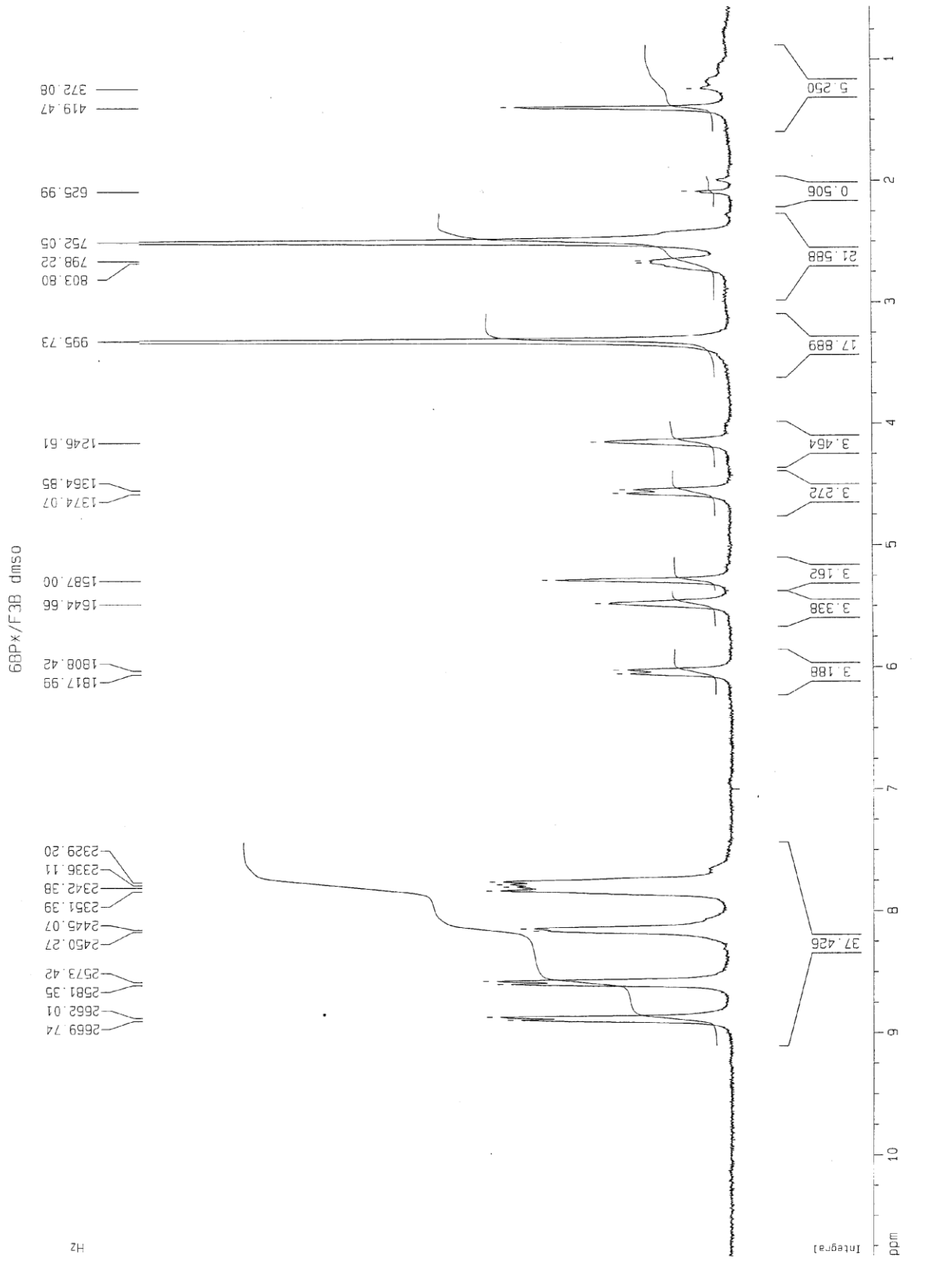
6a

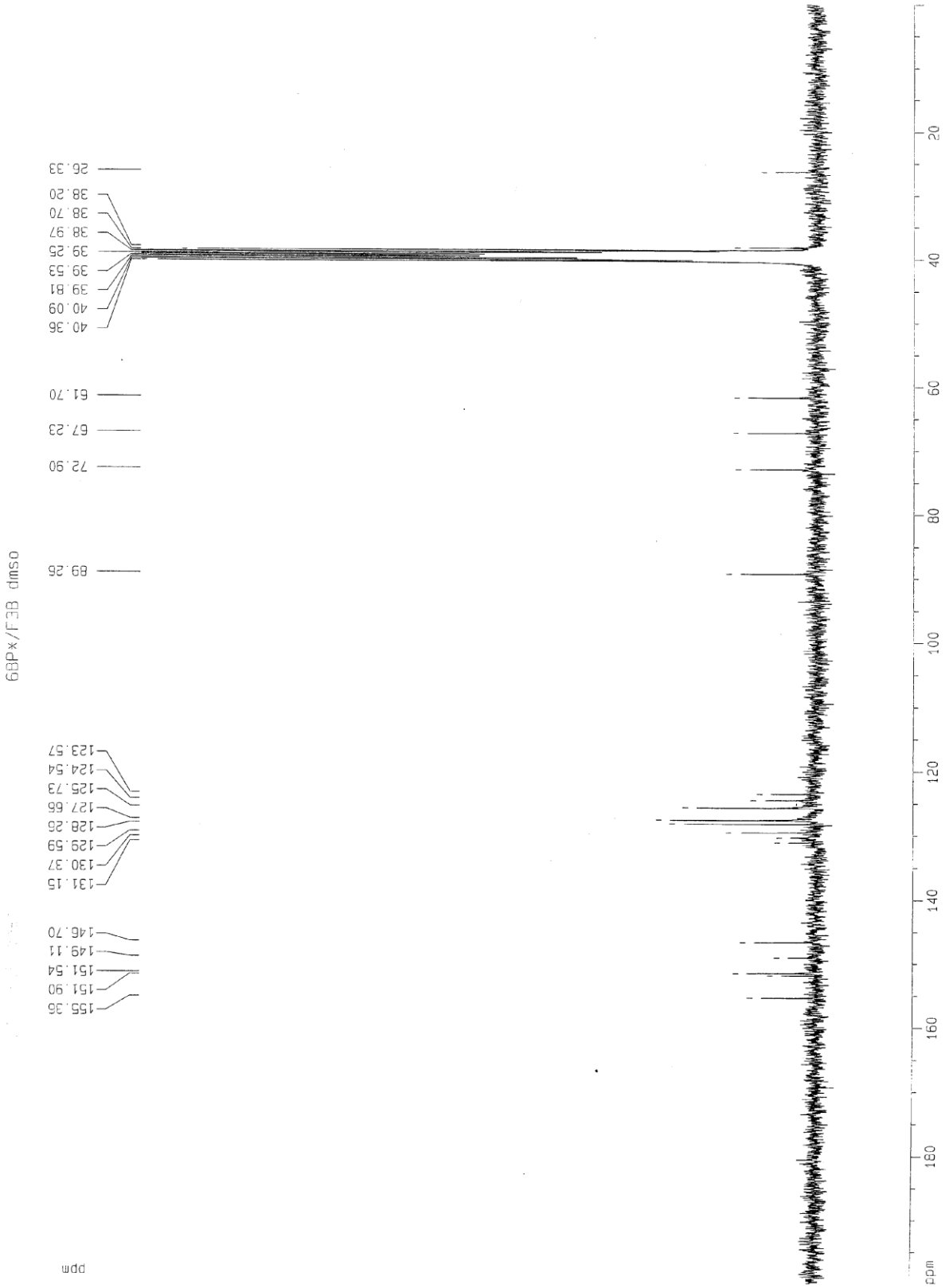

SAR 6A dmso
HZ
ppm
Integral
369.79
687.01
712.35
727.41
751.97
770.51
776.81
782.81
791.15
1005.53
1382.63
1431.86
1435.35
1438.29
1526.54
1534.53
1536.13
1557.30
1566.99
2267.59
2274.19
2282.11
2289.92
2295.74
2313.62
2326.81
2335.32
2341.77
2386.72
2415.45
2417.85
2434.21
2441.63
2446.11
2455.08
2482.51
2556.34
2565.02
2570.22
2576.17
2632.71
-0.199
50.471
6.501
3.013
5.407
0.428
33.591
0.789


SAR-6A dmso
37.80
38.11
38.69
38.97
39.25
39.53
39.81
40.09
40.36
40.77
57.19
57.39
62.93
63.27
76.56
76.68
92.02
92.19
121.56
123.12
124.54
124.70
125.44
125.62
127.32
127.59
127.71
128.00
128.08
128.82
129.34
129.53
130.53
130.72
146.10
146.17
148.37
150.32
150.56
151.01
154.24
154.53
ppm
20
40
60
80
100
120
140
160
180
ppm

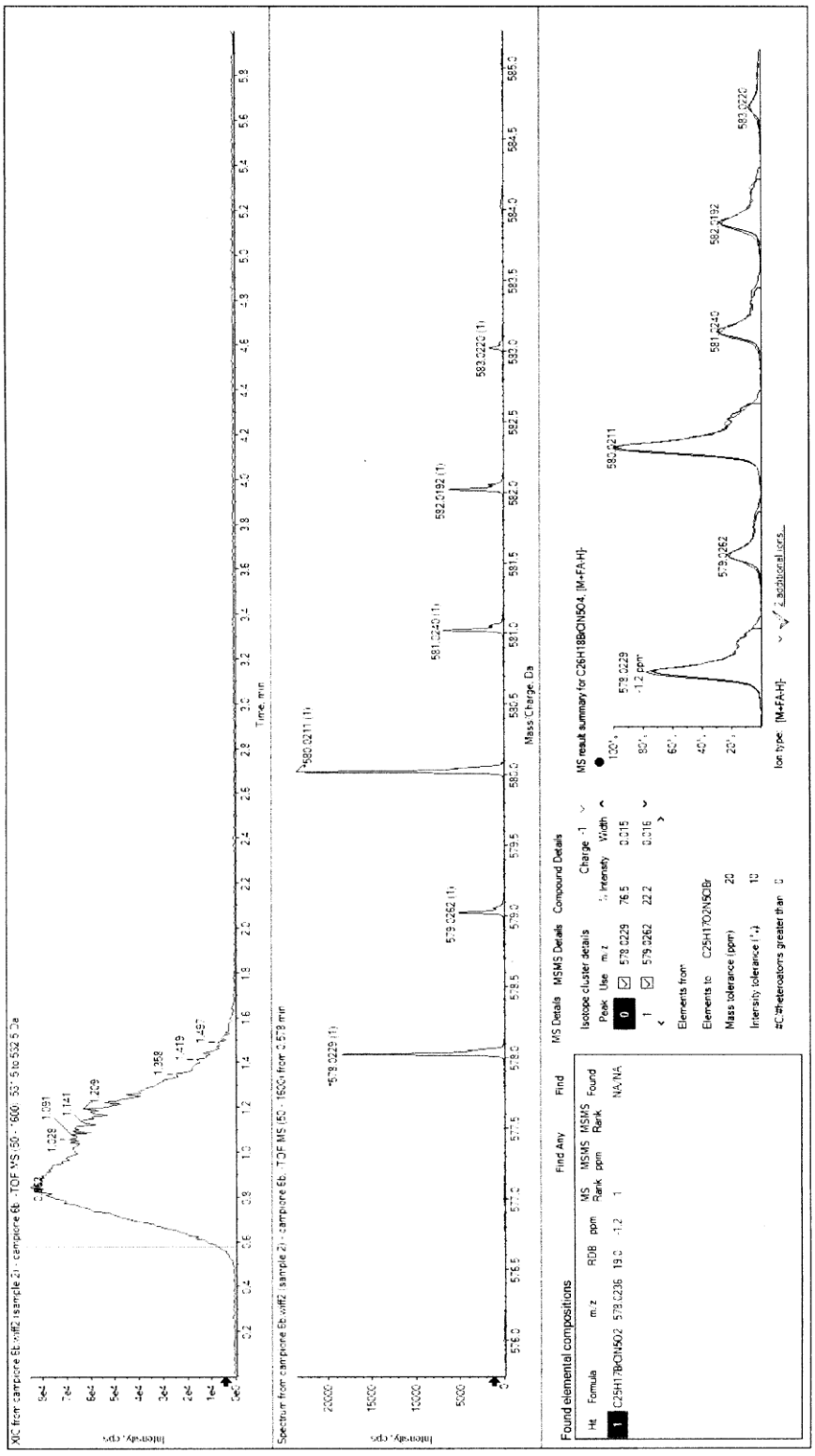

Sample Name
Campione 6a
Formula
C25H17BrClN5O2
Adduct/Charge
[M+FA-H]-
Precursor Mass
578.0236
Found At Mass
578.0238
Mass Error (ppm)
0.3 ppm
Time, min
Mass-Charge, Da
Found elemental compositions
Compound Details
MS result summary for C26H18BrClN5O4 [M-FA-H]
Ion type: [M-FA-H]-

6b

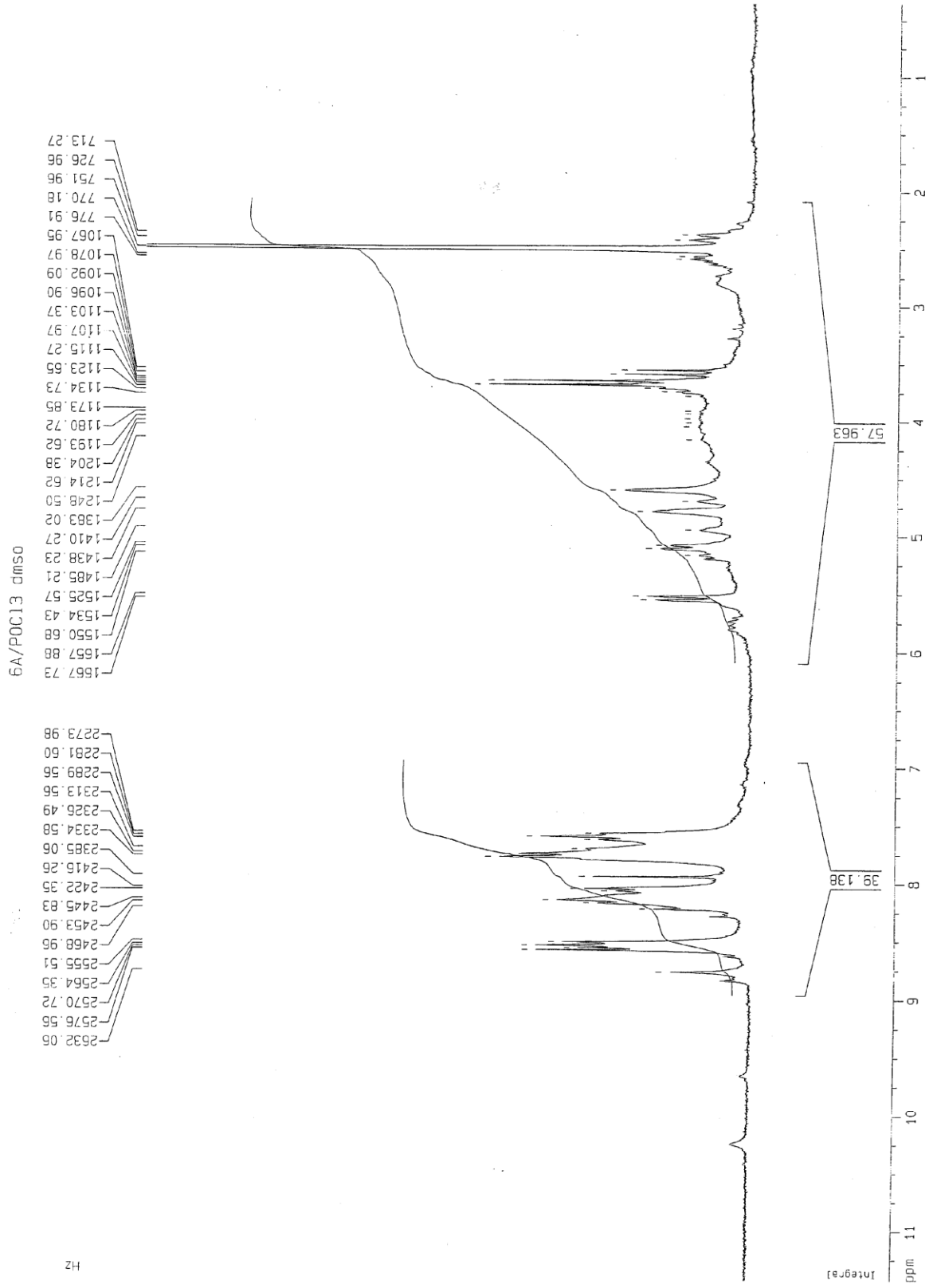

6BPx/F3B dmso
372.08
419.47
625.99
752.05
798.22
803.80
995.73
1246.61
1364.85
1374.07
1587.00
1644.66
1808.42
1817.99
2329.20
2336.11
2342.38
2351.39
2445.07
2450.27
2573.42
2581.35
2662.01
2669.74
5.250
0.506
21.588
17.889
3.464
3.272
3.162
3.338
3.188
37.426
Integral
ppm
H2

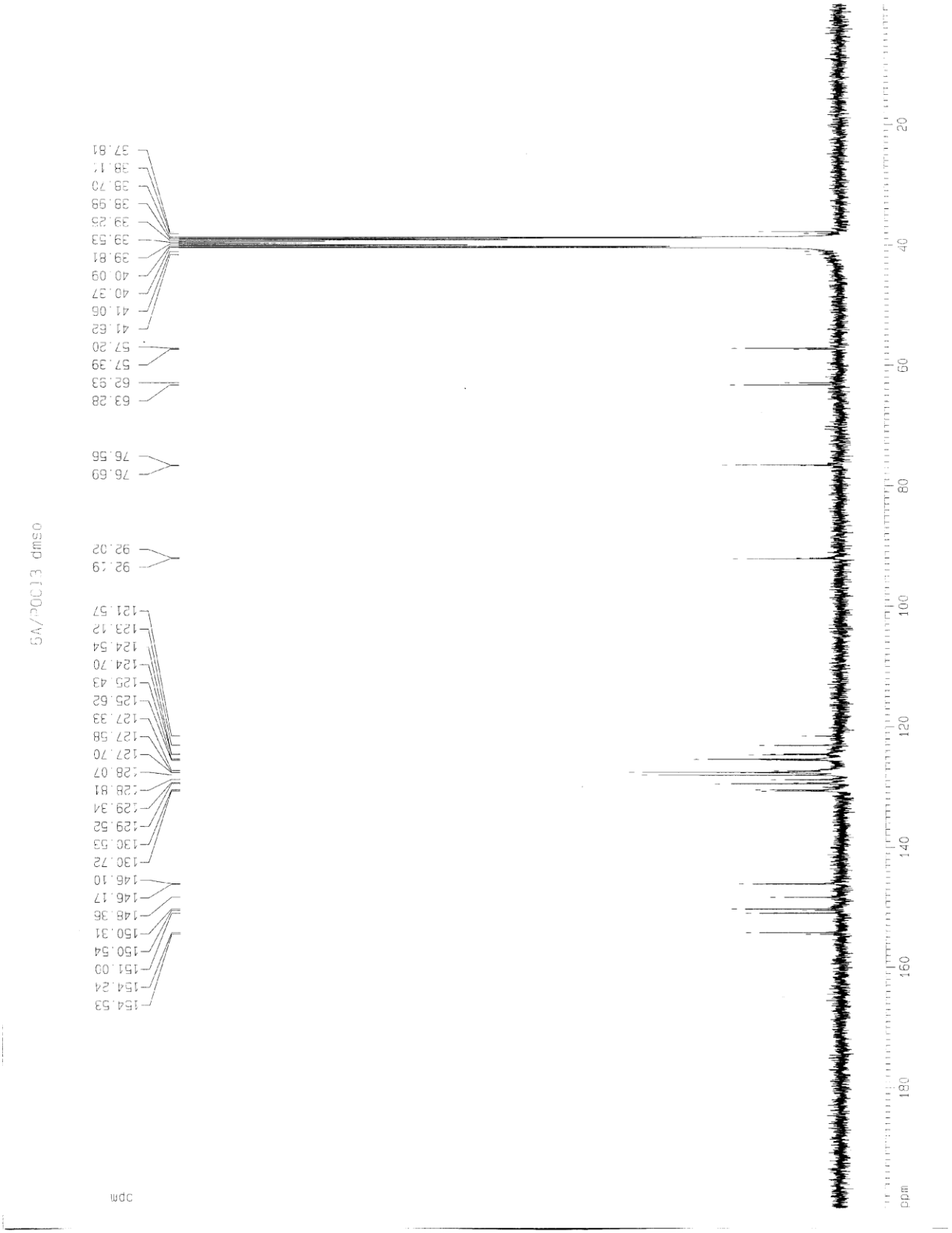

26.33
38.20
38.70
38.97
39.25
39.53
39.81
40.09
40.36
61.70
67.23
72.90
89.26
123.57
124.54
125.73
127.66
128.26
129.59
130.37
131.15
146.70
149.11
151.54
151.90
155.36
GBPx/CDCl3 dmso
ppm
20
40
60
80
100
120
140
160
180
ppm

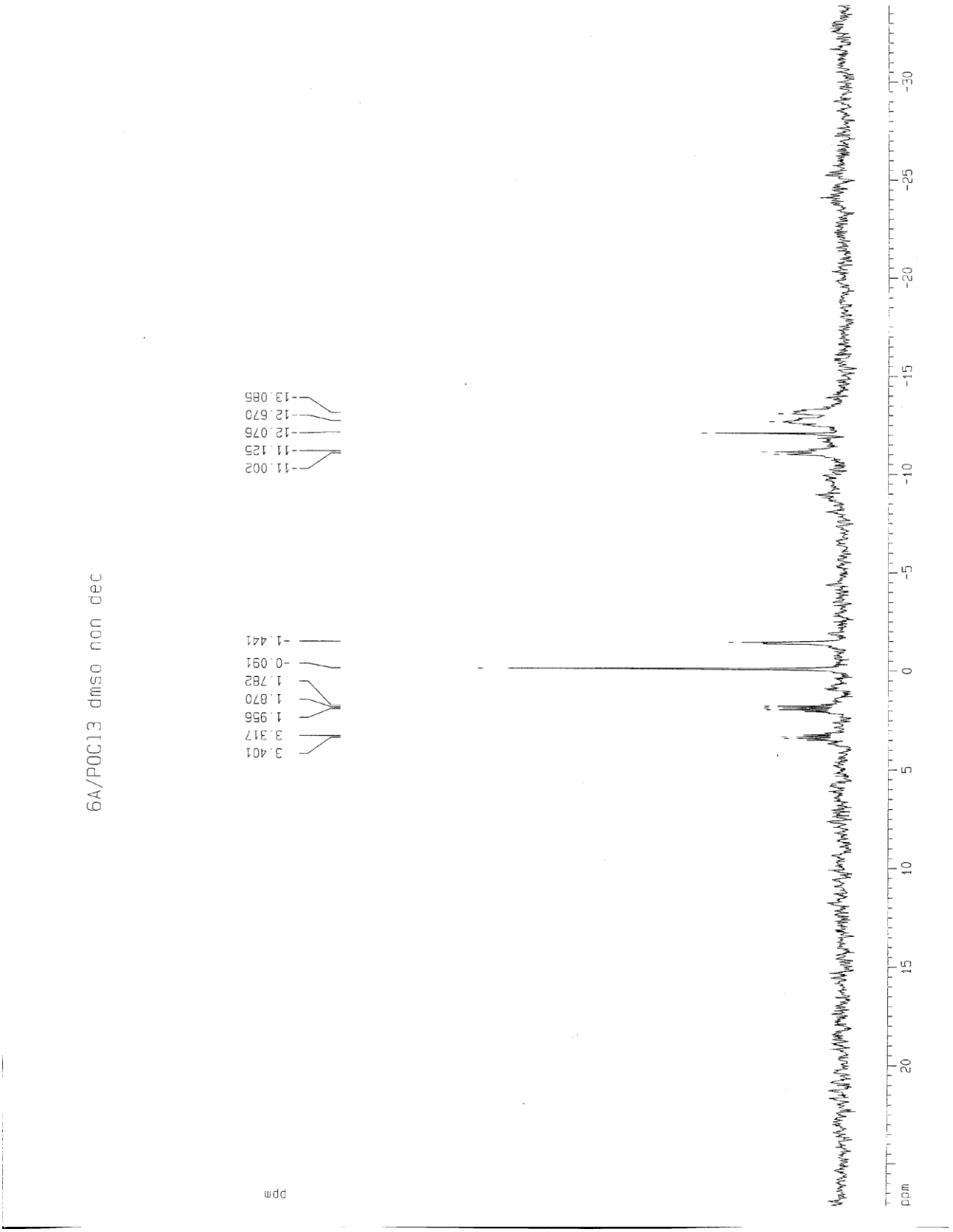
Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Camplone 6b	C25H17BrClNSO2	[M+FA-H]-	578.0236	578.0229	-1.2 ppm



7aA

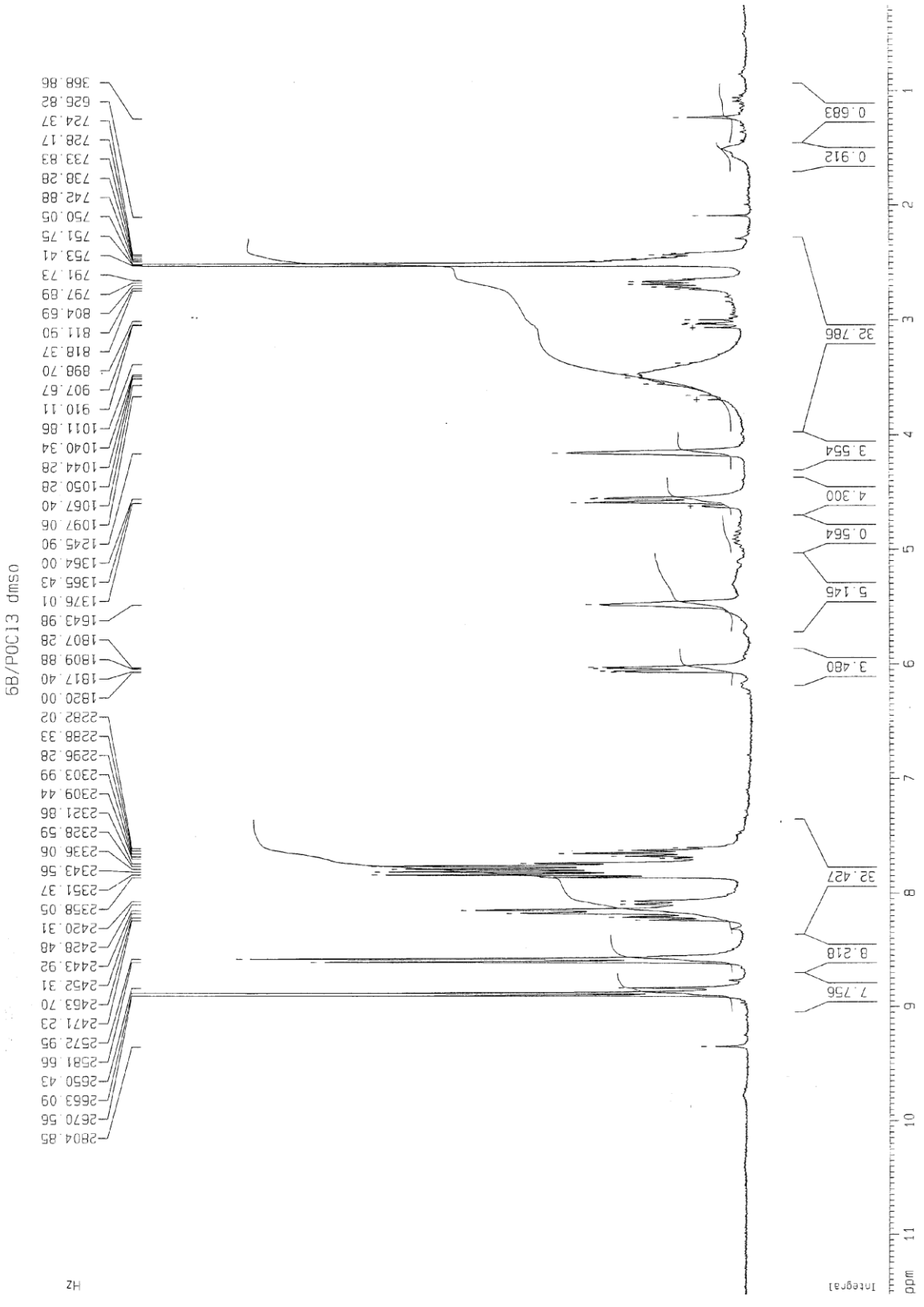

6A/POC13 dmso
713.27
726.96
751.96
770.18
776.91
1067.95
1078.97
1092.09
1096.90
1103.37
1107.97
1115.27
1123.65
1134.73
1173.85
1180.72
1193.62
1204.38
1214.62
1248.50
1383.02
1410.27
1438.23
1485.21
1525.57
1534.43
1550.68
1657.88
1667.73
2273.98
2281.60
2289.56
2313.56
2326.49
2334.58
2385.06
2415.26
2422.35
2445.83
2453.90
2468.96
2555.51
2564.35
2570.72
2576.56
2632.06
57.963
39.138
Integral
ppm
Hz

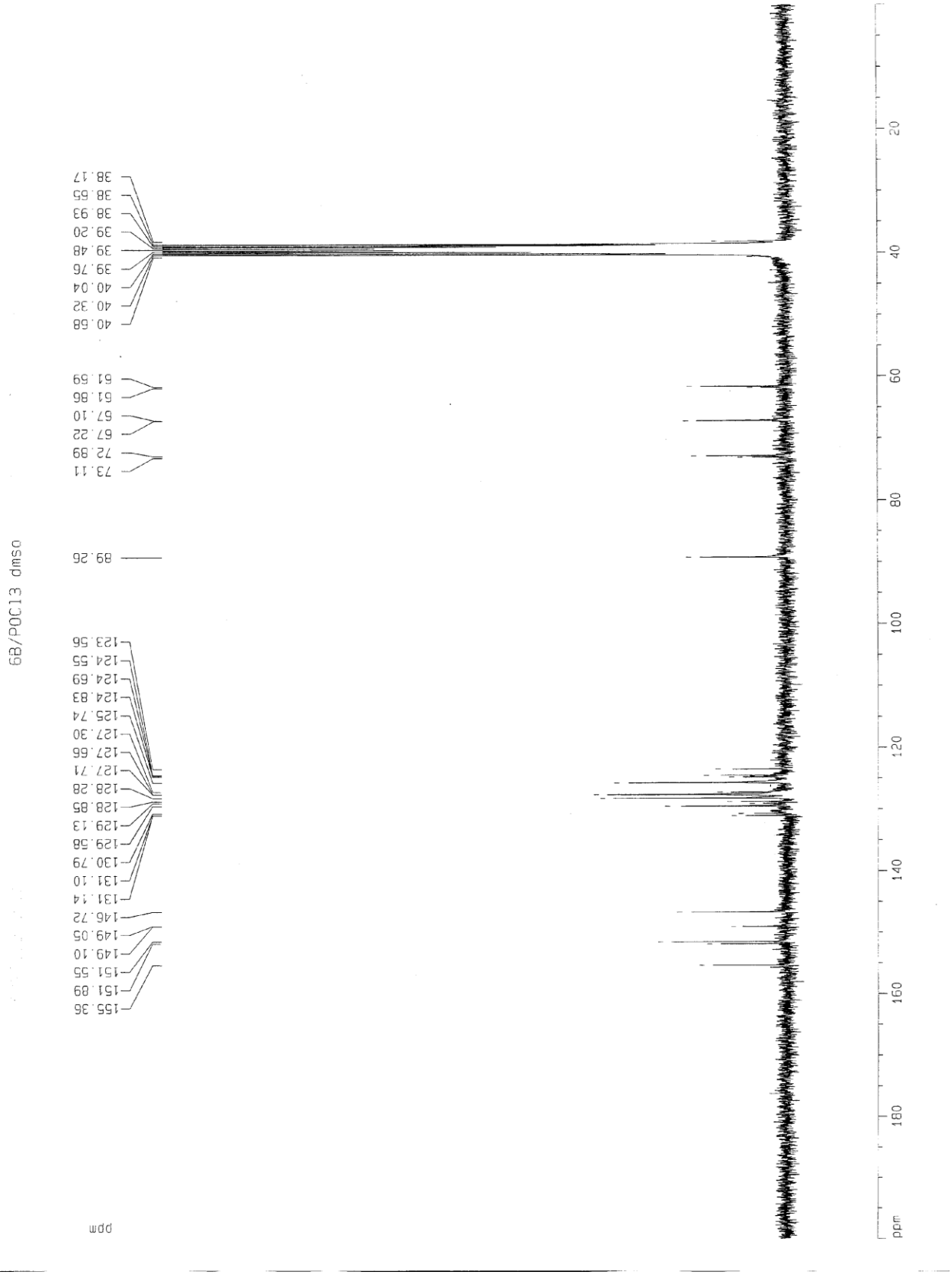

37.81
38.17
38.70
38.99
39.25
39.53
39.81
40.09
40.37
41.06
41.62
57.20
57.39
62.93
63.28
76.56
76.69
92.02
92.29
121.57
123.12
124.54
124.70
125.43
125.62
127.33
127.58
127.70
128.07
128.81
129.34
129.52
130.53
130.72
146.10
146.17
148.36
150.31
150.54
151.00
154.24
154.53
SA/20C13 dmso
wdc
ppm
20
40
60
80
100
120
140
160
180

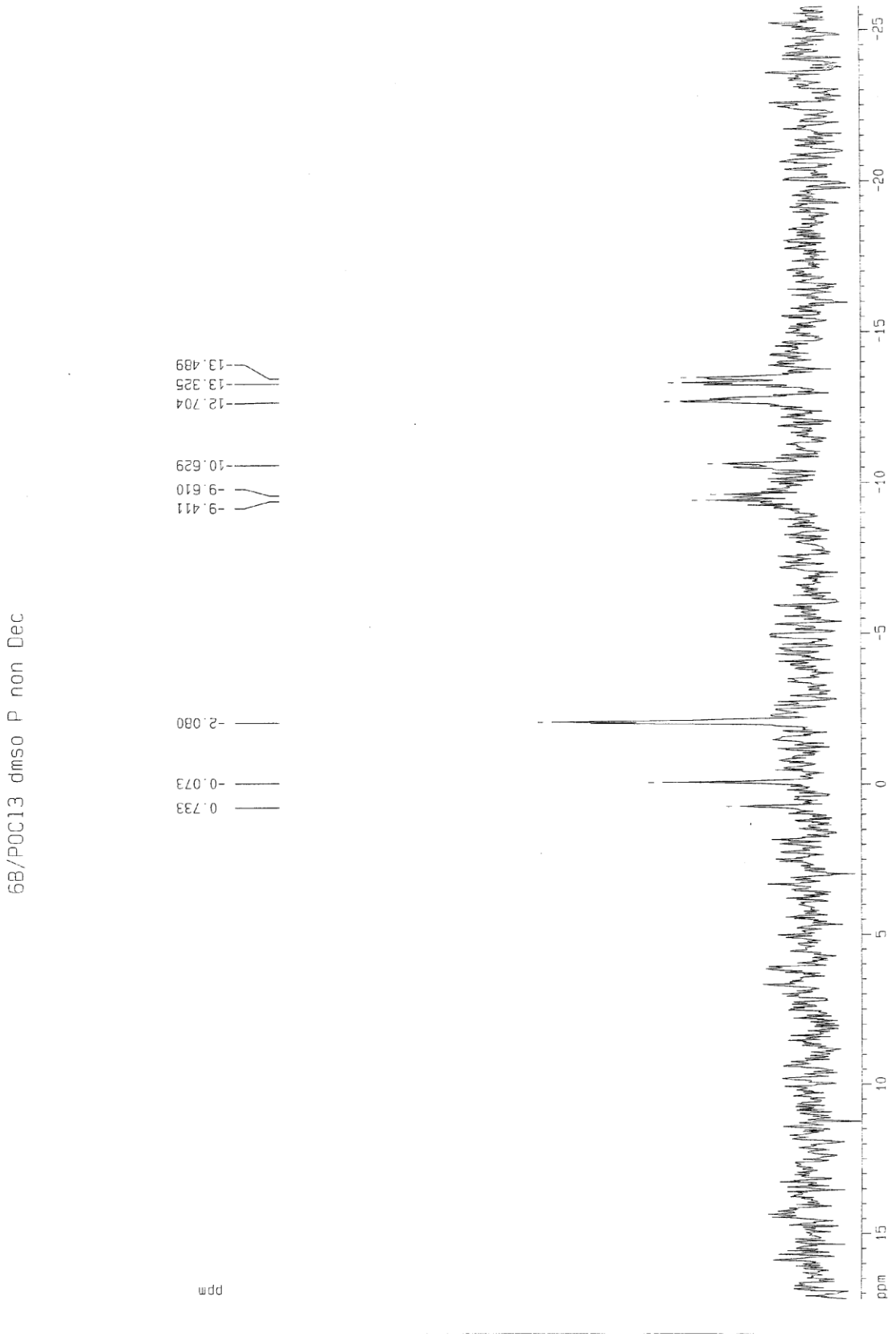

6A/POC13 dmso non dec
3.401
3.317
1.956
1.870
1.782
0.091
-1.441
-11.002
-11.125
-12.076
-12.670
-13.085
ppm
ppm

Sample Name
Campione 6A/POCl3
Formula
C25H18BrClN5O5P
Adduct/Charge
[M-H]-
Precursor Mass
611.9845
Found At Mass
611.9836
Mass Error (ppm)
-1.4 ppm
Intensity, cps
Time, min
Mass/Charge, Da
611.9836 (1)
612.9867 (1)
614.9851 (1)
615.9796 (1)
615.9421 (1)
Found elemental compositions
Hit Formula m/z RDB ppm MS Rank MSMS ppm MSMS Rank Found
1 C25H19BrClN5O5P 611.9845 19.0 -1.4 1 NA NA
Isotope cluster details
Peak Use m/z % Intensity Width
0 611.9836 65.5 0.219
1 612.9867 16.7 0.220
Elements from
Elements to C25H19BrClN5O5P
Mass tolerance (ppm) 20
Intensity tolerance (+/-) 10
#C #heteroatoms greater than 0
MS result summary for C25H17BrClN5O5P, [M-H]-
611.9836
-1.4 ppm
Ion type: [M-H]-
3 additional ions

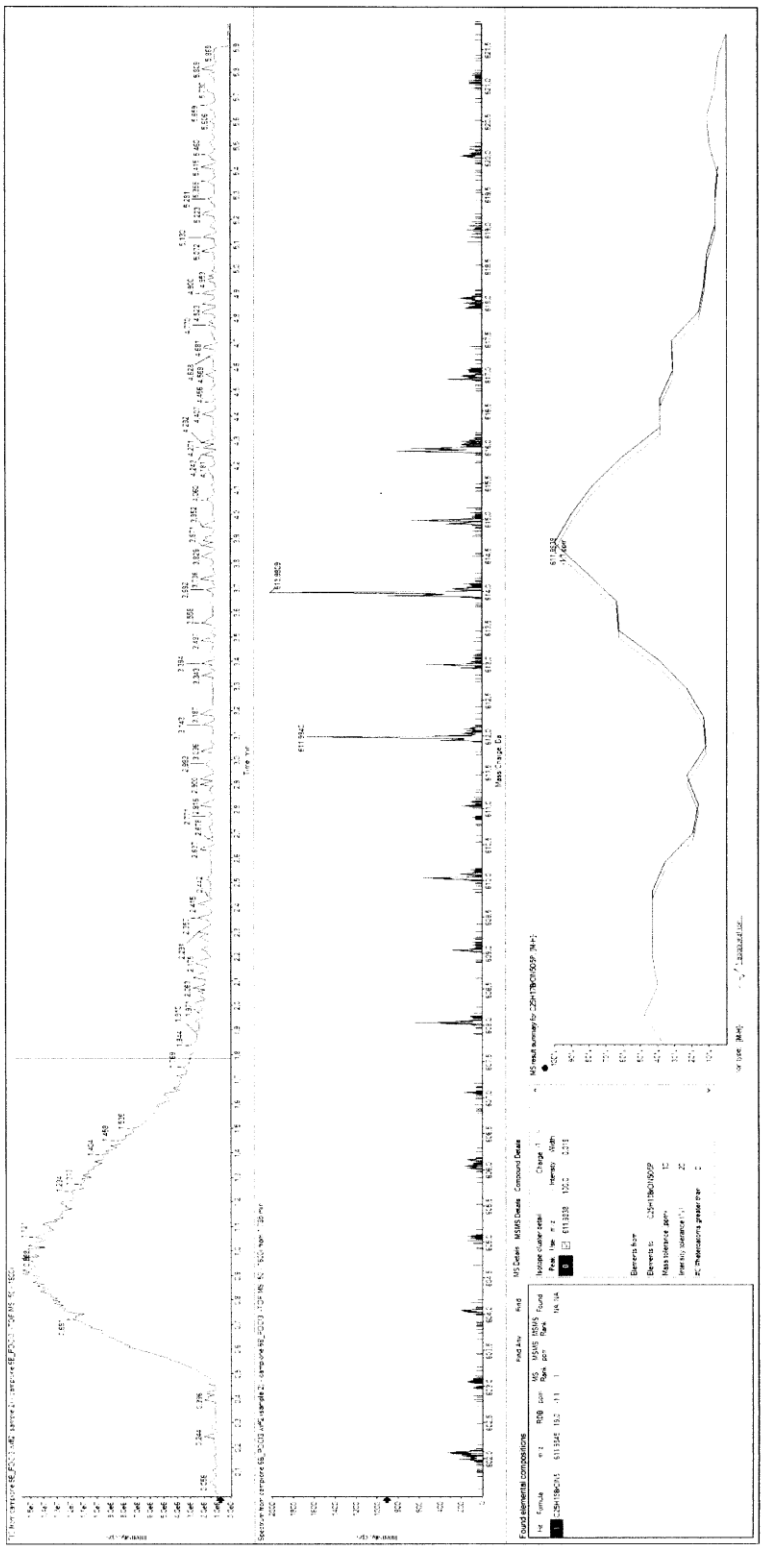
7aB


6B/POC13 dmso
Hz
Integral
ppm
0.683
0.912
32.786
3.554
4.300
0.564
5.145
3.480
32.427
8.218
7.756

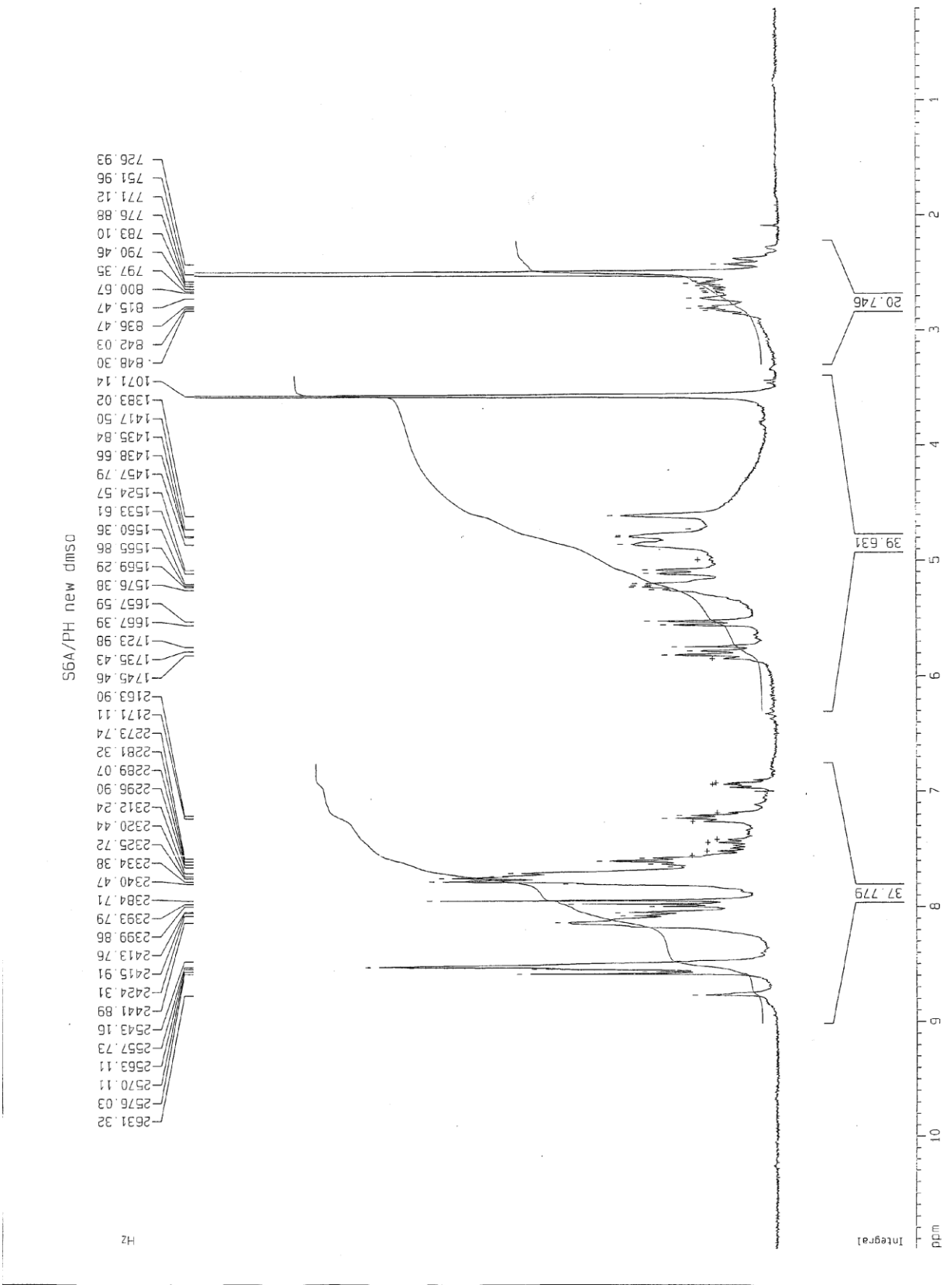

6B/POC13 dmso
38.17
38.55
38.93
39.20
39.48
39.76
40.04
40.32
40.58
51.59
51.86
67.10
67.22
72.89
73.11
89.26
123.56
124.55
124.69
124.83
125.74
127.30
127.66
127.71
128.28
128.85
129.13
129.58
130.79
131.10
131.14
146.72
149.05
149.10
151.55
151.89
155.36
ppm
20
40
60
80
100
120
140
160
180
ppm

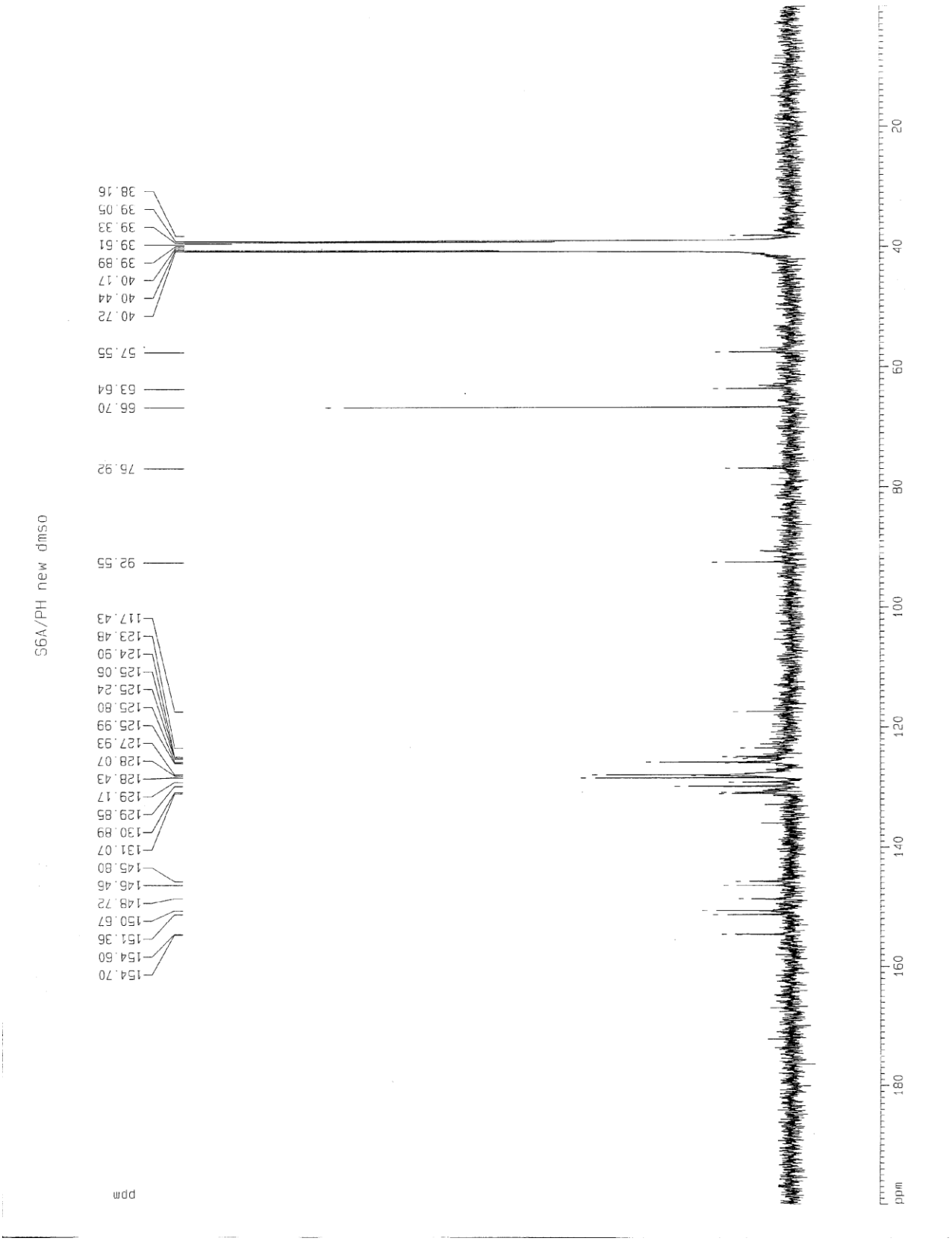

6B/POC13 dmso P non Dec
-13.489
-13.325
-12.704
-10.629
-9.610
-9.411
-2.080
-0.073
0.733
ppm
-25
-20
-15
-10
-5
0
5
10
15
ppm

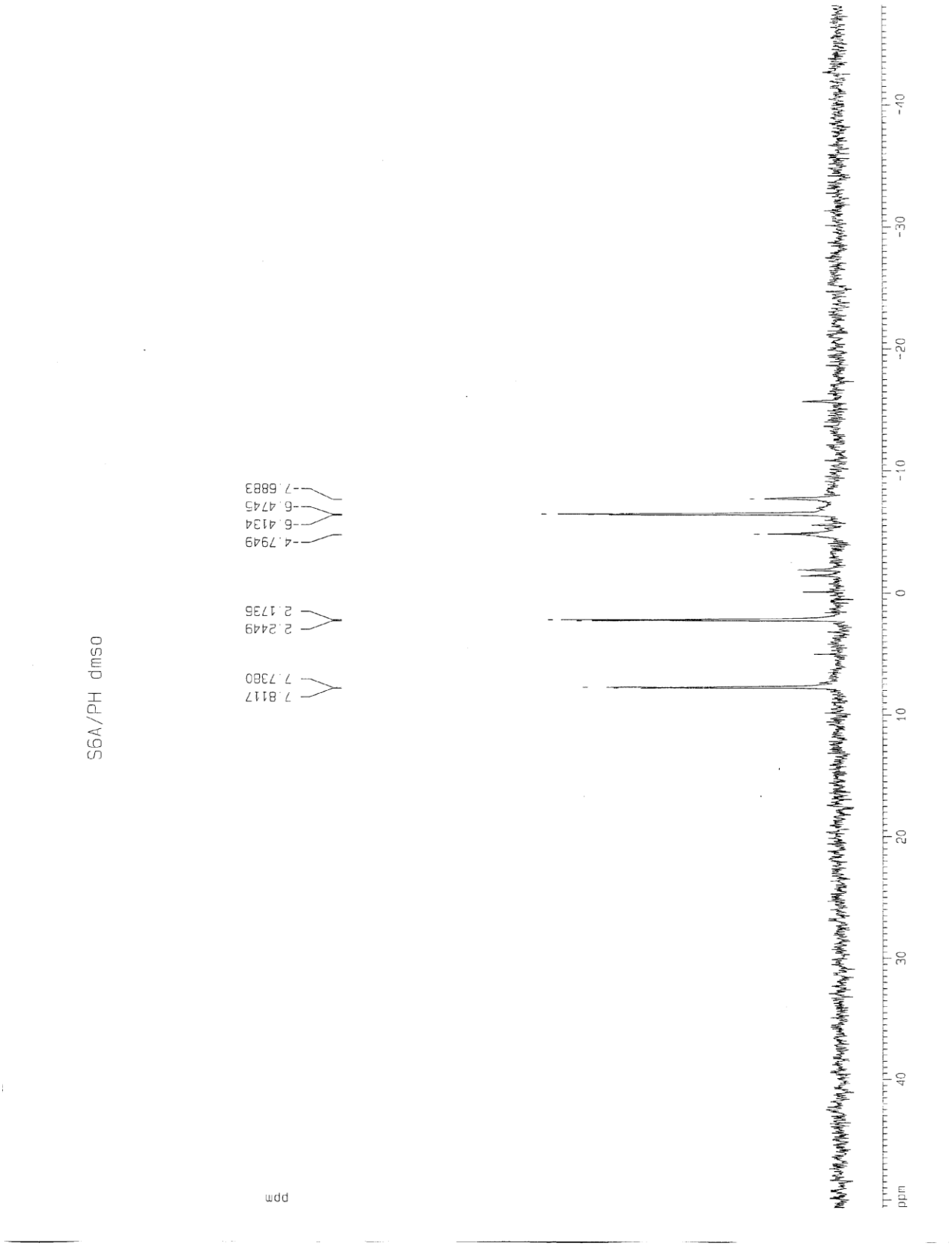
Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 6B/POCl3	C25H18BrClNSO5P	[M-H]-	611.9845	611.9836	-1.4 ppm

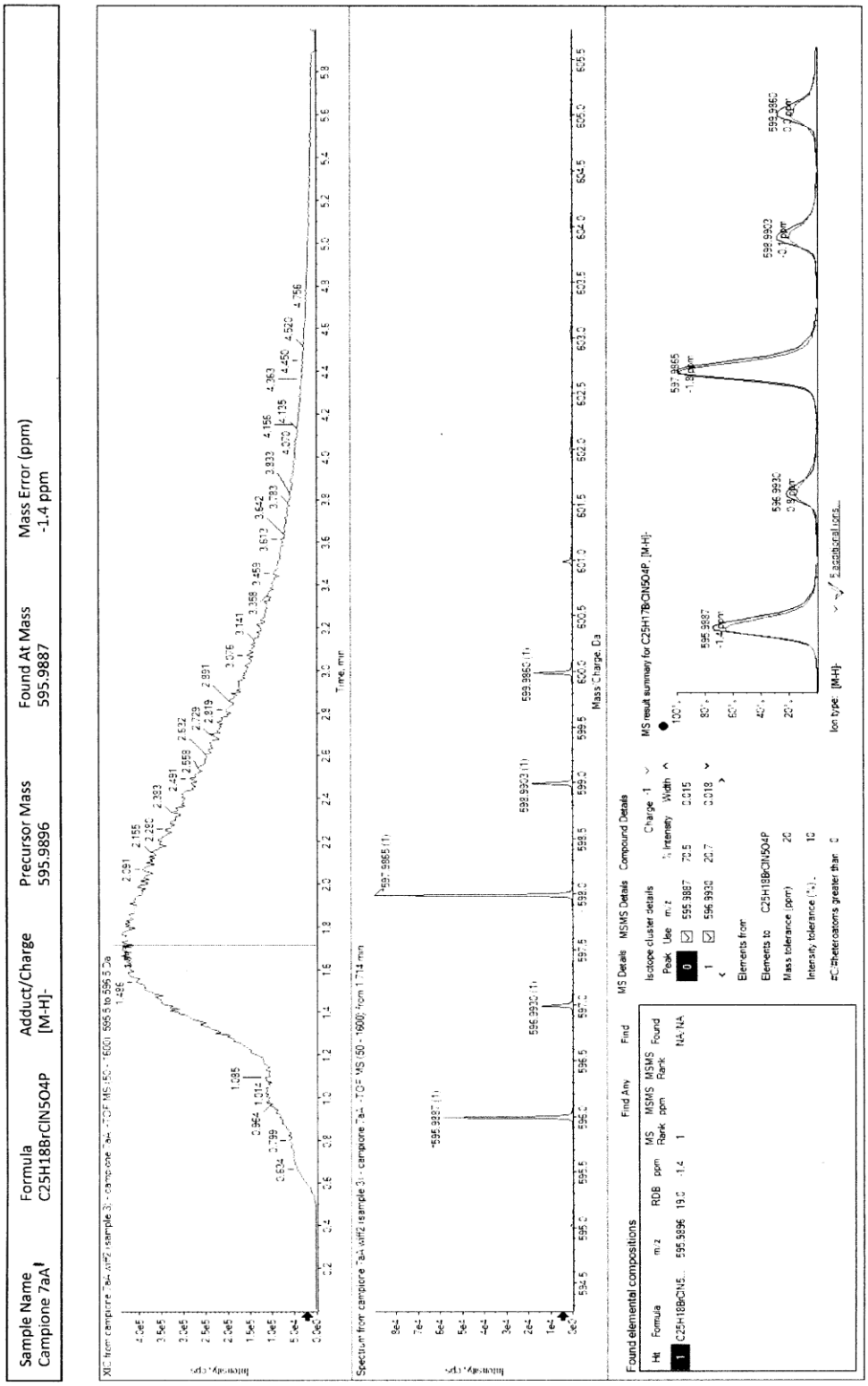


7bA

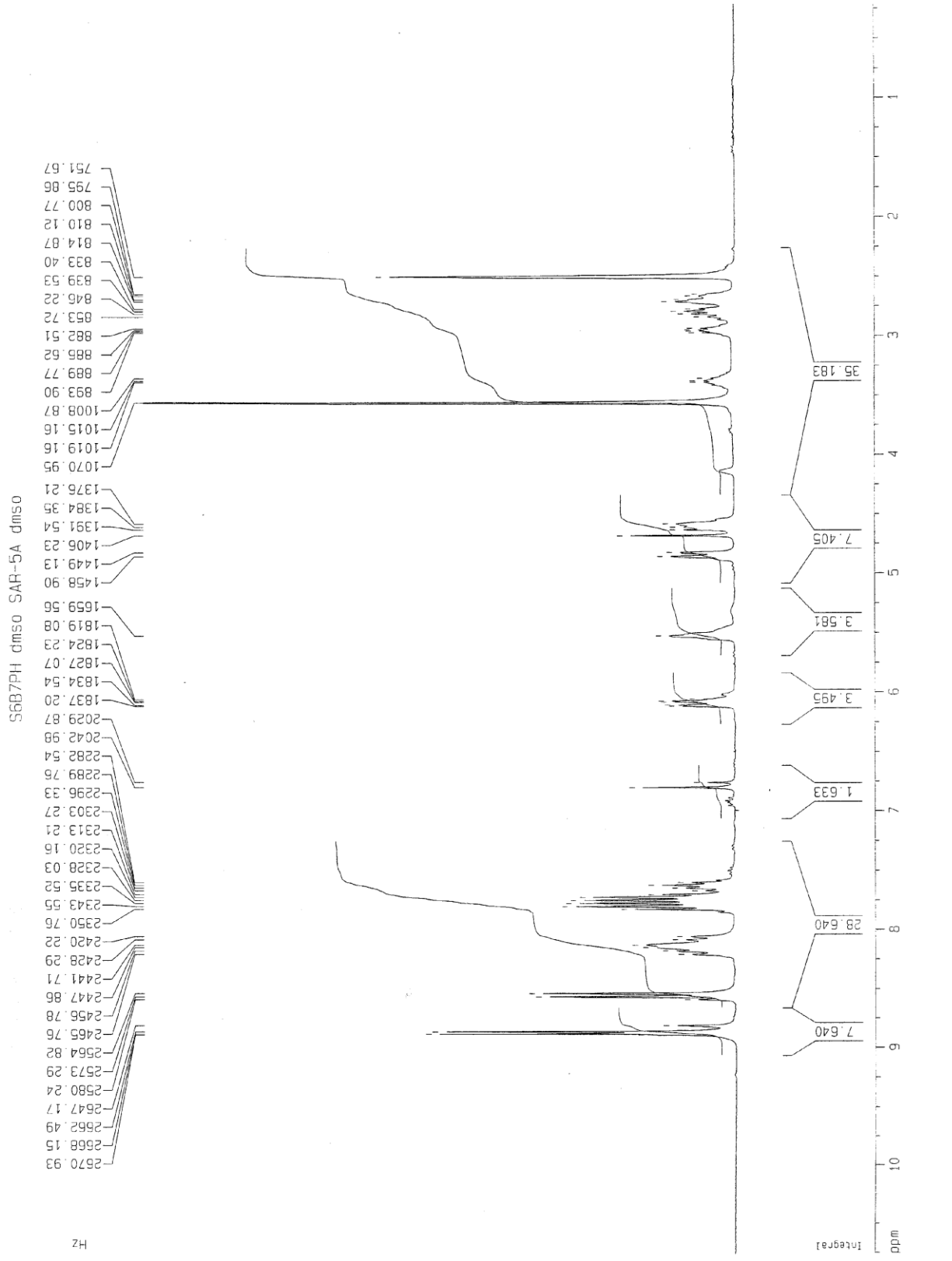

S6A/PH new dmso
7826.93
7751.96
7711.12
7766.88
7783.10
7790.46
7797.35
8000.67
8015.47
8036.47
8042.03
8048.30
10711.14
13830.02
14117.50
14350.84
14386.66
14577.79
15240.57
15336.61
15603.36
15555.86
15592.29
15763.38
16573.59
16673.39
17239.98
17354.43
17454.46
21630.90
21711.11
22737.74
22813.32
22890.07
22960.90
23122.24
23202.44
23257.72
23343.38
23400.47
23841.71
23937.79
23990.86
24137.76
24159.91
24243.31
24418.89
25431.16
25573.73
25631.11
25701.11
25763.03
26311.32
H2
Integral
ppm
20.746
39.631
37.779

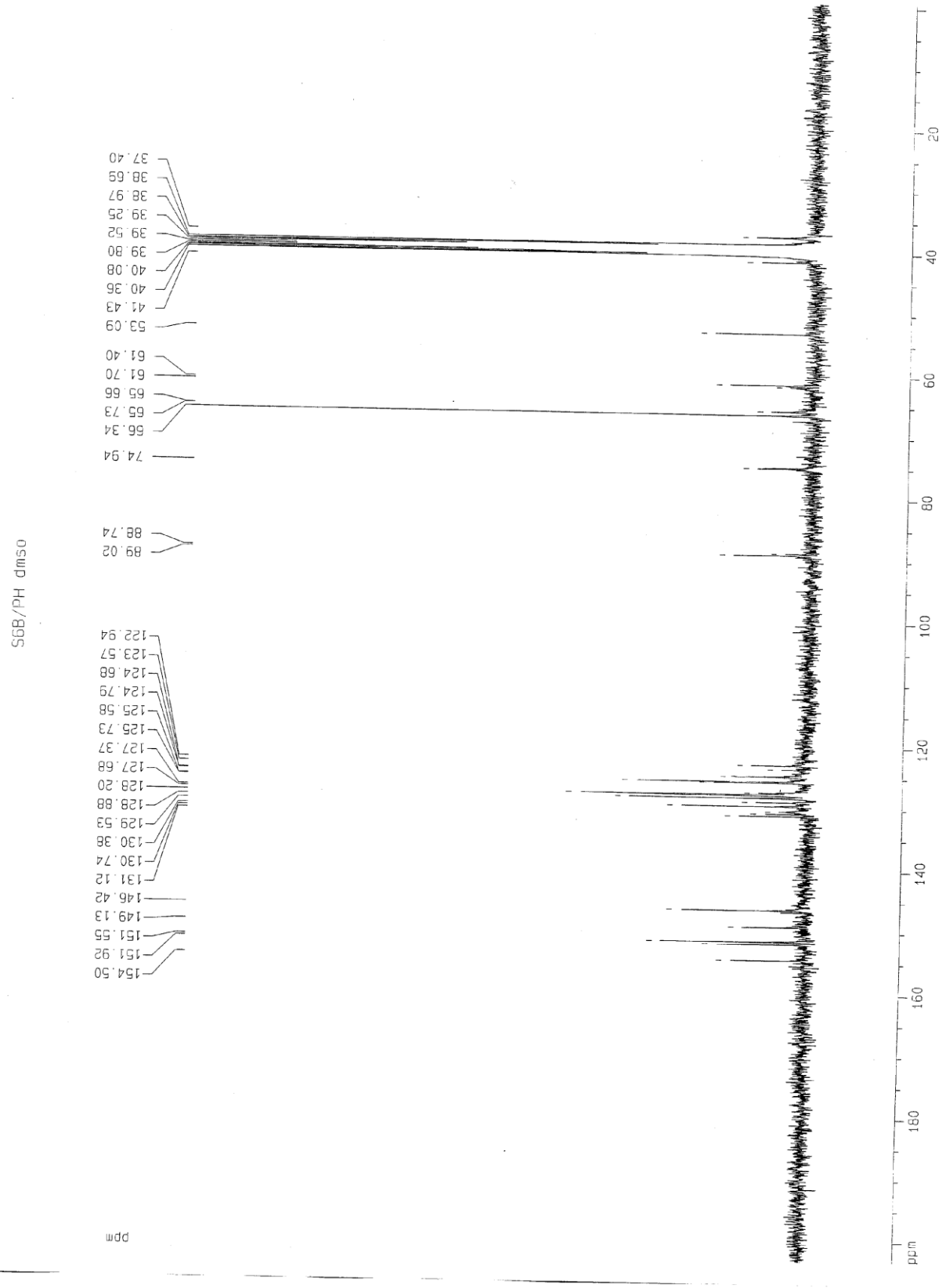

SGA/PH new dmso
38.16
39.05
39.33
39.61
39.89
40.17
40.44
40.72
57.55
63.64
66.70
76.92
92.55
117.43
123.48
124.90
125.05
125.24
125.80
125.99
127.93
128.07
128.43
129.17
129.85
130.89
131.07
145.80
146.46
148.72
150.67
151.36
154.60
154.70
ppm
20
40
60
80
100
120
140
160
180
ppm

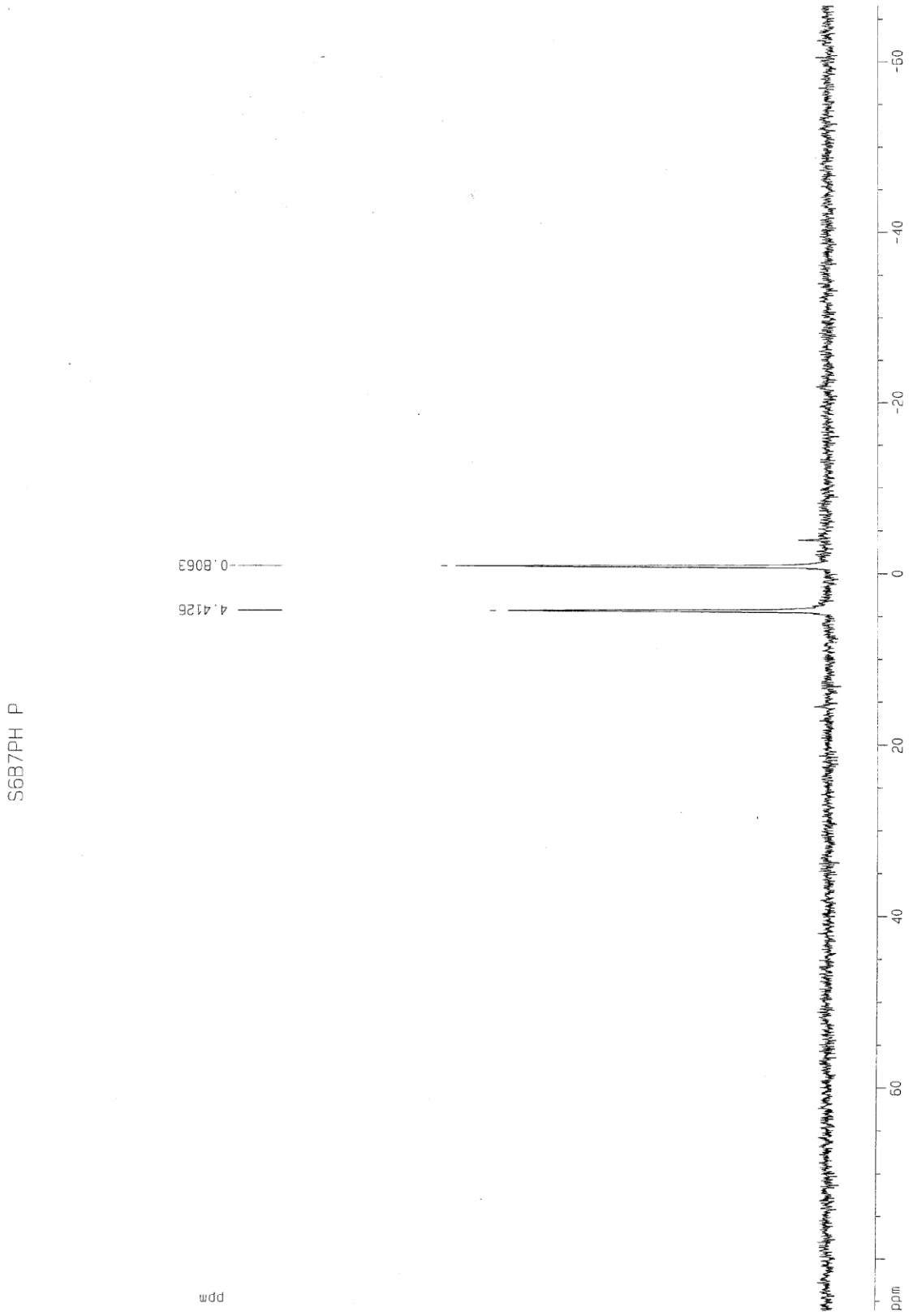

SGA/PH dmso
7.8117
7.7380
2.2449
2.1735
-4.7949
-6.4134
-6.4745
-7.6883
ppm
40
30
20
10
0
-10
-20
-30
-40

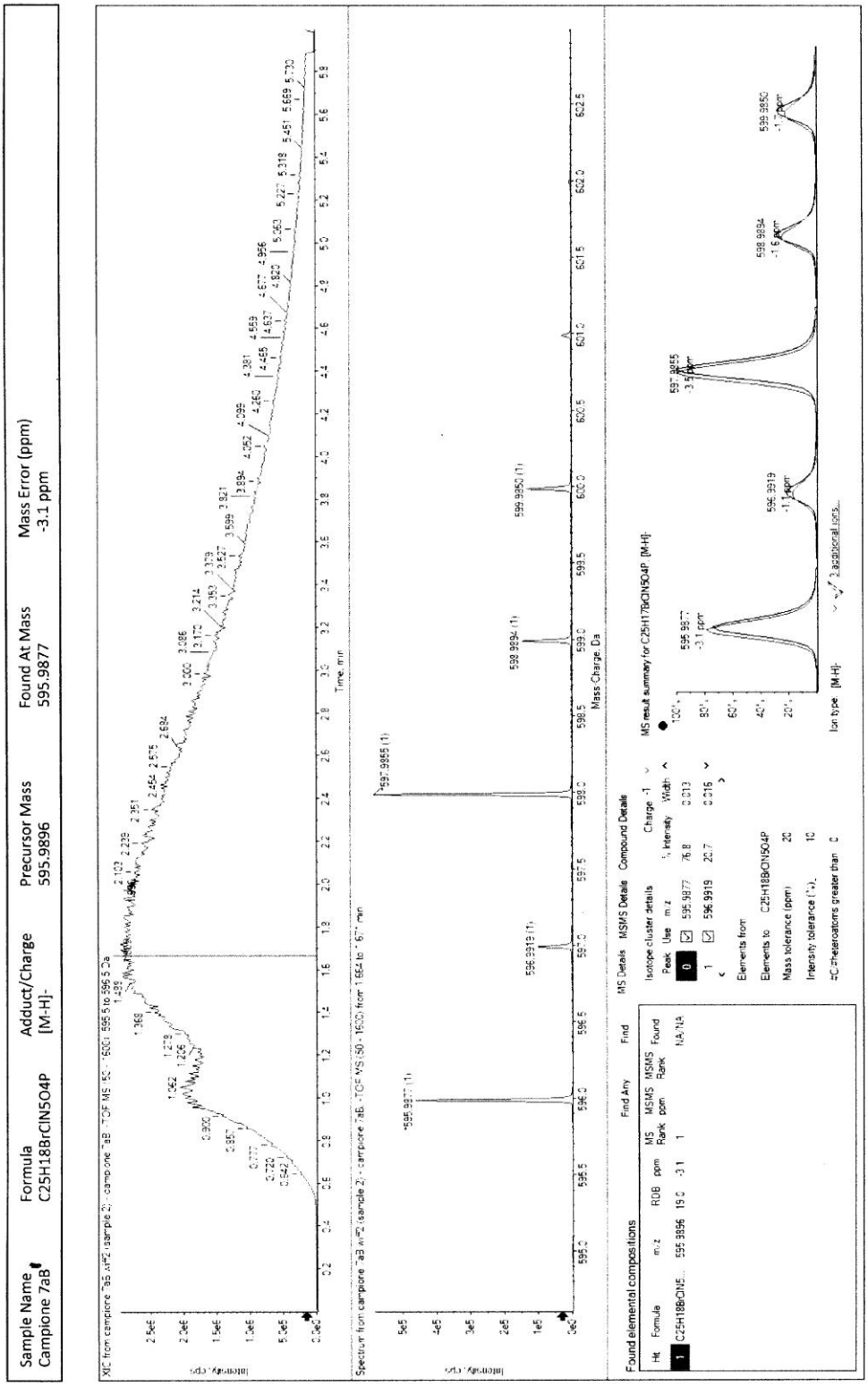

Sample Name
Campione 7aA
Formula
C25H18BrClN5O4P
Adduct/Charge
[M-H]-
Precursor Mass
595.9896
Found At Mass
595.9887
Mass Error (ppm)
-1.4 ppm
Found elemental compositions
Hit Formula m/z RDB ppm MS Rank MSMS ppm MSMS Rank Found
1 C25H18BrClN5... 595.9896 19.0 -1.4 1 NA NA
MS Details MSMS Details Compound Details
Isotope cluster details
Peak Use m/z % Intensity Width
0 595.9887 78.5 0.015
1 596.9930 20.7 0.018
Elements from
Elements to C25H18BrClN5O4P
Mass tolerance (ppm) 20
Intensity tolerance (%) 10
#C #heteroatoms greater than 0
MS result summary for C25H17BrClN5O4P [M-H]-
595.9887
-1.4 ppm
596.9930
0.9 ppm
597.9865
-1.8 ppm
598.9903
0.1 ppm
598.9960
0.7 ppm
Ion type: [M-H]-
Add/delete ions...

7bB

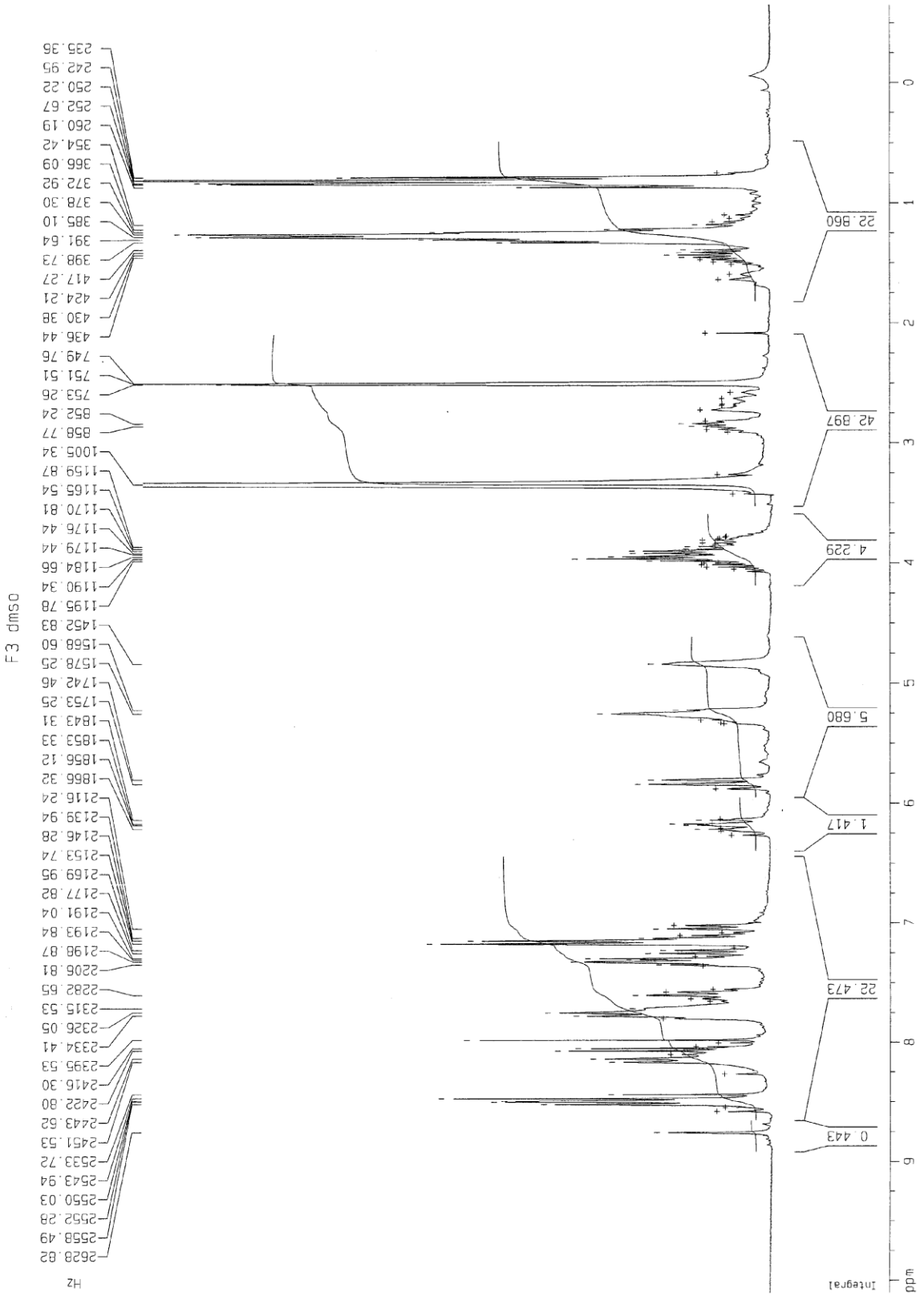

S6B7PH dmso SAR-5A dmso
Hz
Integral
ppm
35.183
7.405
3.581
3.495
1.633
28.640
7.640

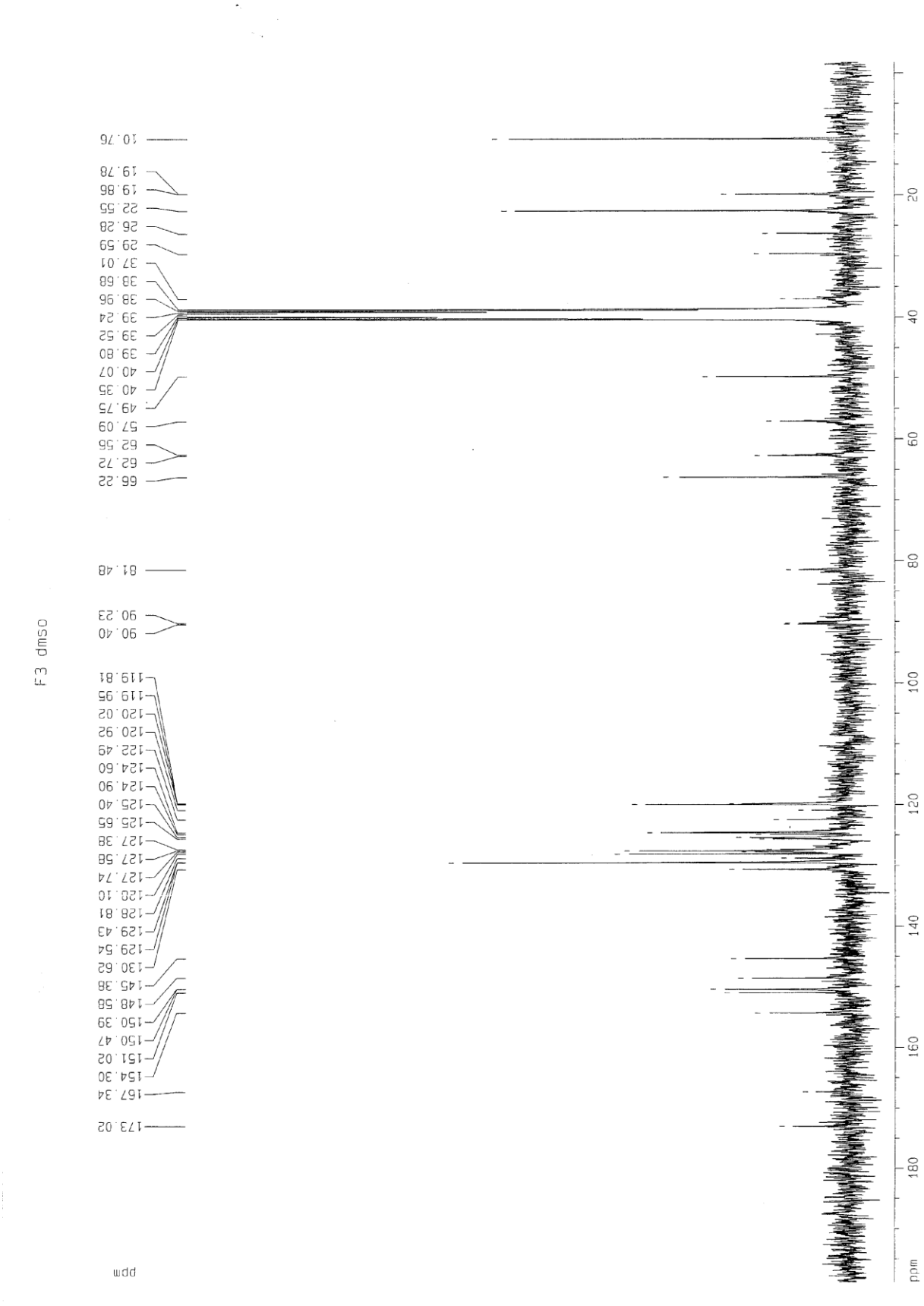

37.40
38.69
38.97
39.25
39.52
39.80
40.08
40.36
41.43
53.09
61.40
61.70
65.66
65.73
66.34
74.94
88.74
89.02
122.94
123.57
124.68
124.79
125.58
125.73
127.37
127.68
128.20
128.88
129.53
130.38
130.74
131.12
146.42
149.13
151.55
151.92
154.50
S6B/PH dmso
ppm
20
40
60
80
100
120
140
160
180
ppm

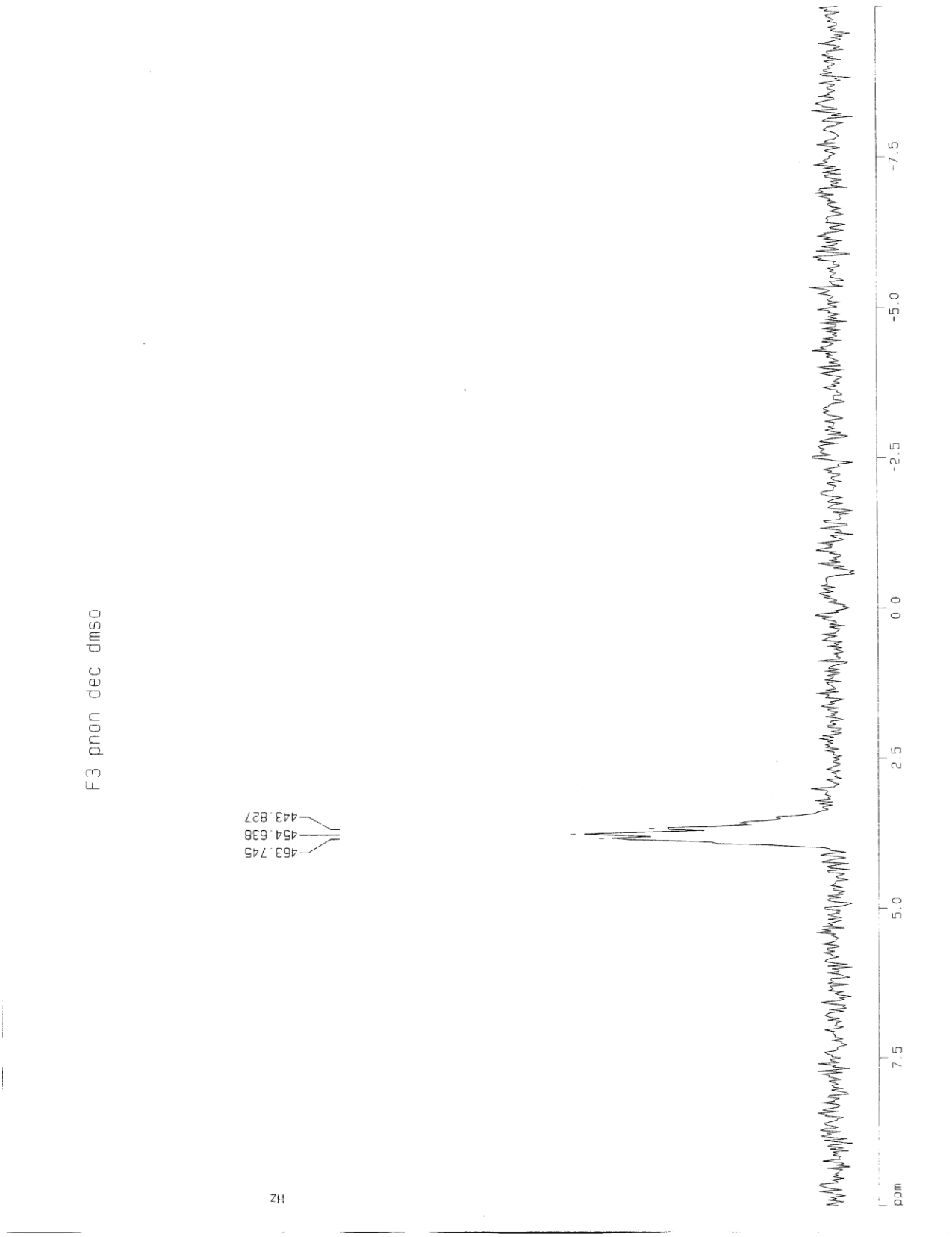



Sample Name
Campione 7aB
Formula
C25H18BrClN5O4P
Adduct/Charge
[M-H]-
Precursor Mass
595.9896
Found At Mass
595.9877
Mass Error (ppm)
-3.1 ppm
Found elemental compositions
Hit
Formula
m/z
RDB
ppm
MS Rank
MSMS ppm
MSMS Rank
Found
C25H18BrClN5...
595.9896
19.0
-3.1
1
N/A
N/A
MS Details
MSMS Details
Compound Details
Find Any
Find
Isotope cluster details
Charge -1
Peak
Use
m/z
% Intensity
Width
MS result summary for C25H17BrClN5O4P [M-H]-
Elements from
Elements to C25H18BrClN5O4P
Mass tolerance (ppm) 20
Intensity tolerance (+/-) 10
Ion type [M-H]-
2 additional ions...
Time, min
Mass Charge, Da
Intensity, CPS

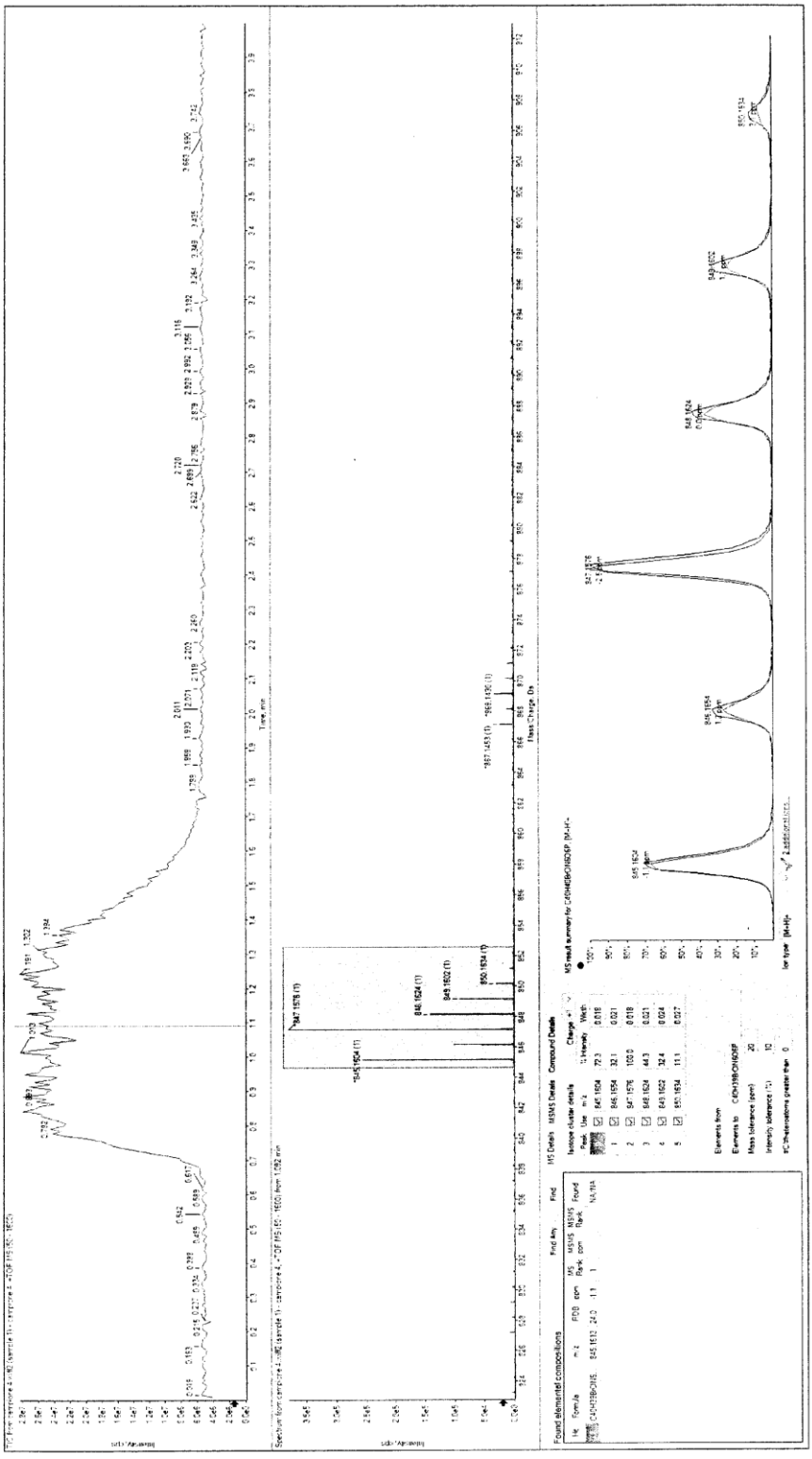
7cA


F3 dmso
Hz
2628.82
2558.49
2552.28
2550.03
2543.94
2533.72
2451.53
2443.62
2422.80
2416.30
2395.53
2334.41
2326.05
2315.53
2282.65
2206.81
2198.87
2193.84
2191.04
2177.82
2169.95
2153.74
2146.28
2139.94
2116.24
1866.32
1856.12
1853.33
1843.31
1753.25
1742.46
1578.25
1568.60
1452.83
1195.78
1190.34
1184.66
1179.44
1176.44
1170.81
1165.54
1159.87
1005.34
858.77
852.24
753.26
751.51
749.76
436.44
430.38
424.21
417.27
398.73
391.64
385.10
378.30
372.92
366.09
354.42
260.19
252.67
250.22
242.95
235.36
Integral
22.860
42.897
4.229
5.680
1.417
22.473
0.443
ppm
0
1
2
3
4
5
6
7
8
9

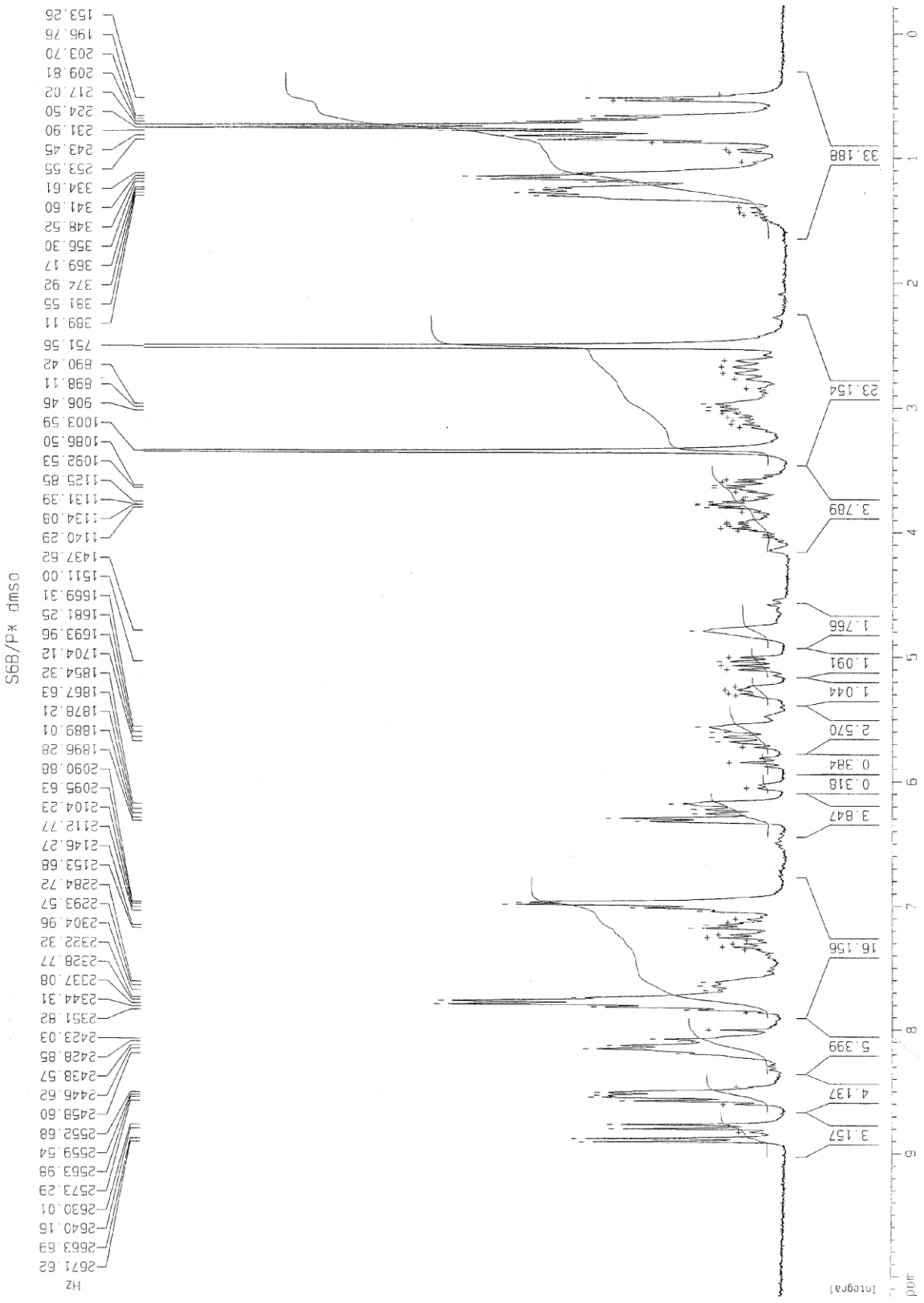

10.76
19.78
19.86
22.55
26.28
29.59
37.01
38.68
38.96
39.24
39.52
39.80
40.07
40.35
49.75
57.09
62.55
62.72
66.22
81.48
90.23
90.40
119.81
119.95
120.02
120.92
122.49
124.60
124.90
125.40
125.65
127.38
127.58
127.74
128.10
128.81
129.43
129.54
130.62
145.38
148.58
150.39
150.47
151.02
154.30
157.34
173.02
DMSO F3
ppm

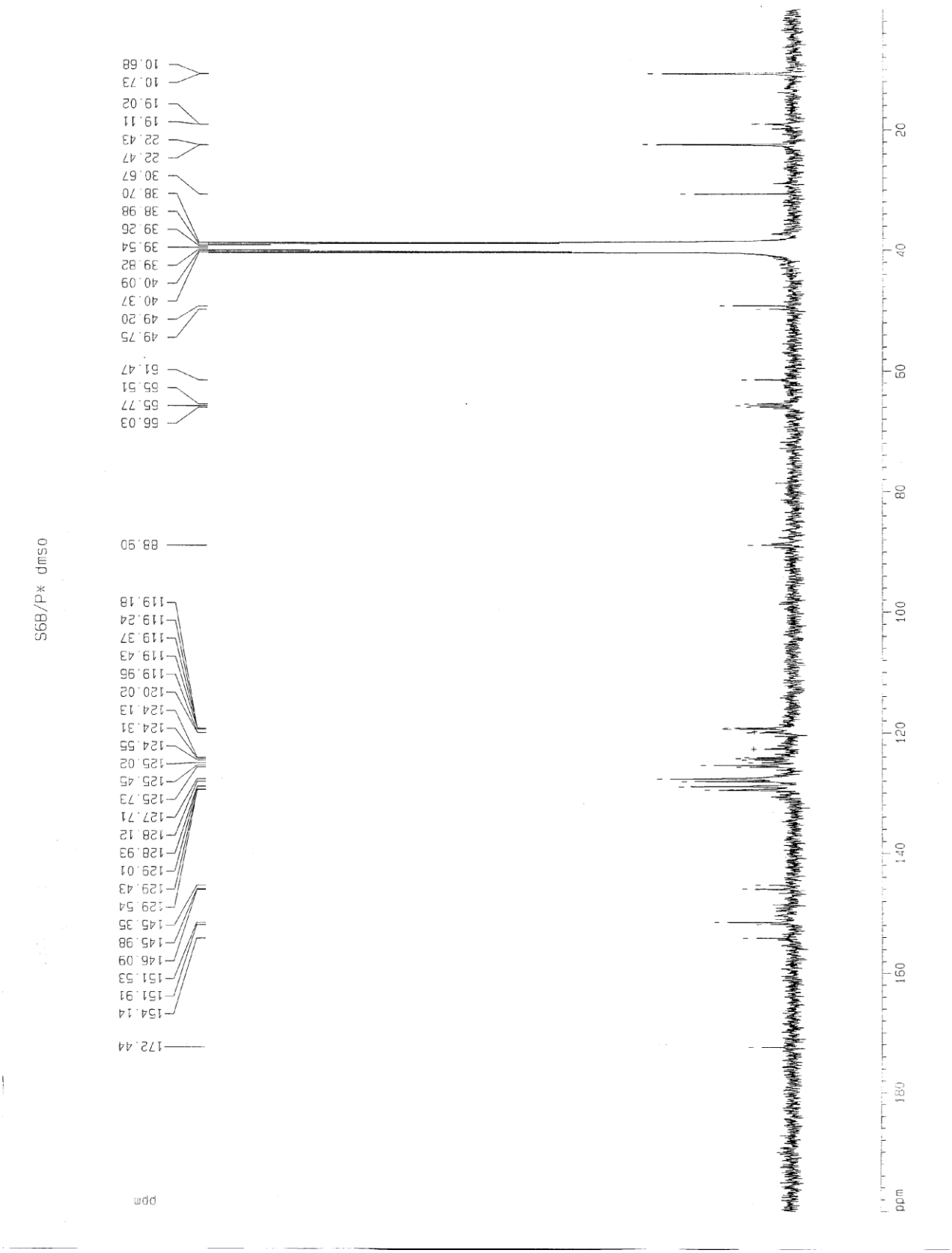

F3 pnon dec dmso
463.745
454.638
443.827
Hz
ppm
7.5
5.0
2.5
0.0
-2.5
-5.0
-7.5

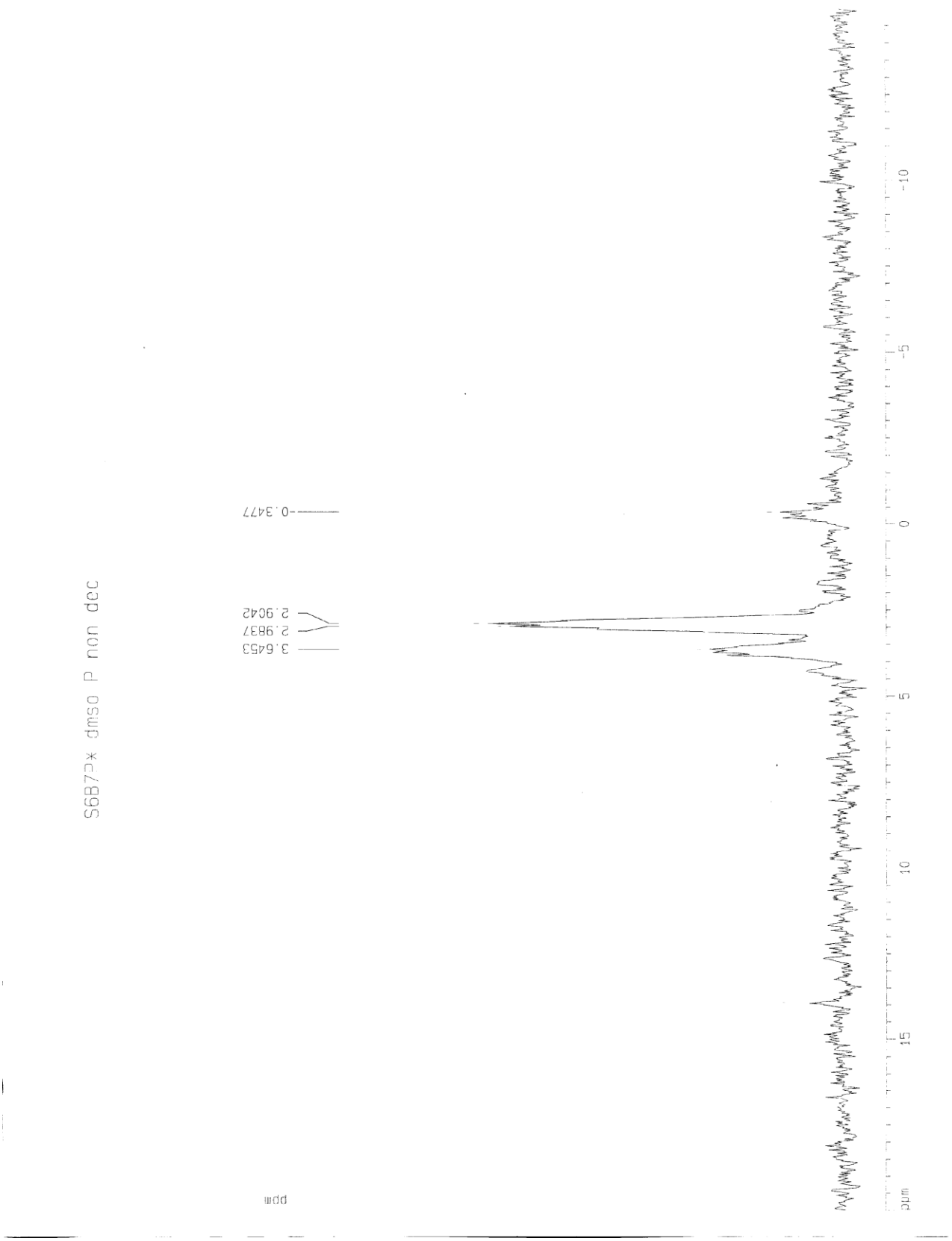
Sample Name	Formula	Adduct / Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Camplone 4	C40H39BrClN6O6P	[M+H]+	845.1613	845.1604	-1.1 ppm



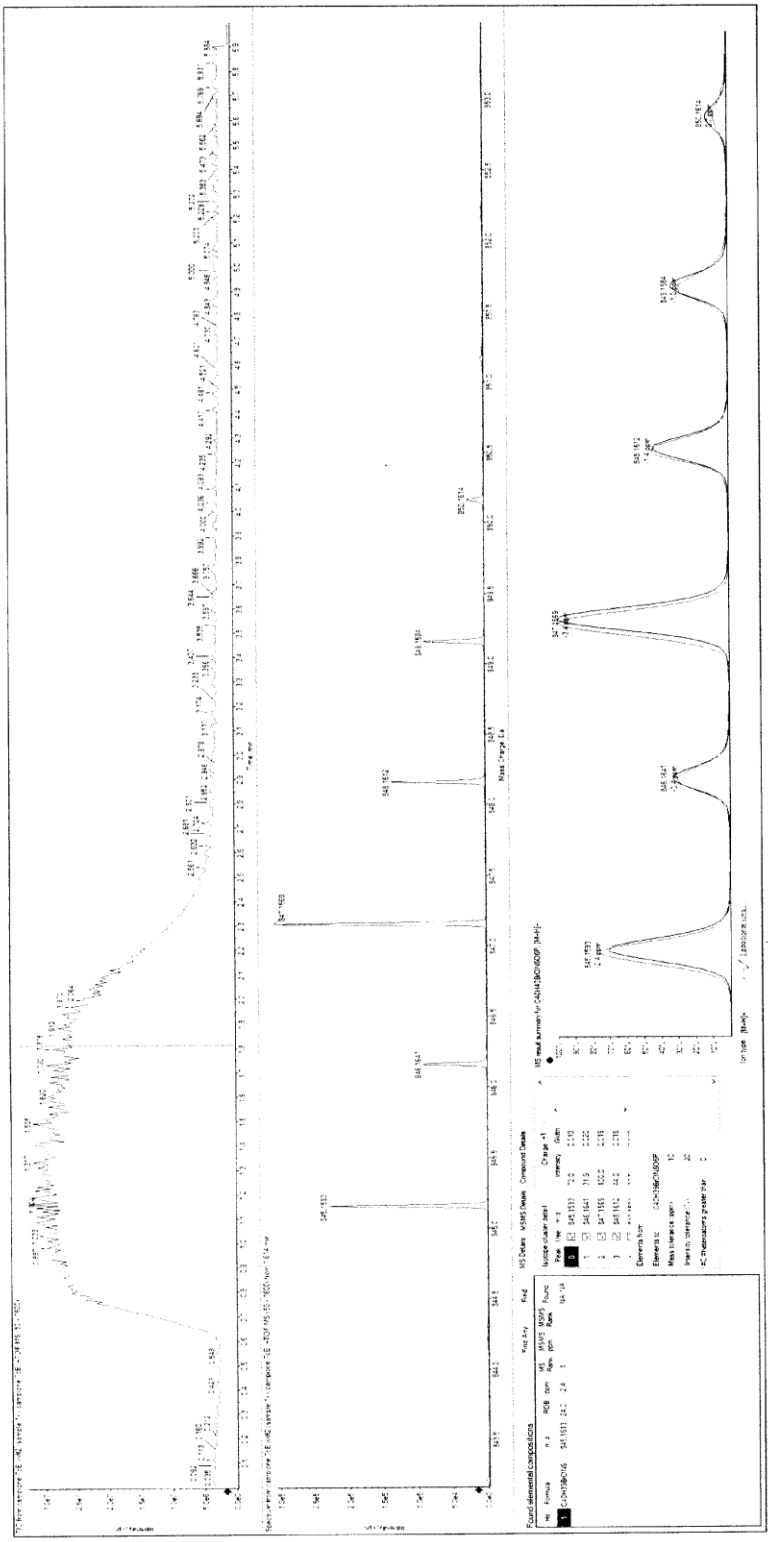
7cB


S6B/P* dmso
Hz
153.26
196.76
203.70
209.81
217.02
224.50
231.90
243.45
253.55
334.61
341.60
348.52
356.30
369.17
374.92
381.55
389.11
751.56
890.42
898.11
906.46
1003.59
1086.50
1092.53
1125.85
1131.39
1134.08
1140.29
1437.62
1511.00
1669.31
1681.25
1693.96
1704.12
1854.32
1867.63
1878.21
1889.01
1896.28
2090.88
2095.63
2104.23
2112.77
2146.27
2153.68
2284.72
2293.57
2304.96
2322.32
2328.77
2337.08
2344.31
2351.82
2423.03
2428.85
2438.57
2446.62
2458.60
2552.68
2559.54
2563.98
2573.29
2630.01
2640.16
2663.69
2671.62
Integral
ppm
33.188
23.154
3.789
1.766
1.091
1.044
2.570
0.384
0.318
3.847
16.156
5.399
4.137
3.157
0
1
2
3
4
5
6
7
8
9


S6B/P* dmso
10.68
10.73
19.02
19.11
22.43
22.47
30.67
38.70
38.98
39.26
39.54
39.82
40.09
40.37
49.20
49.75
51.47
55.51
65.77
66.03
88.90
119.18
119.24
119.37
119.43
119.96
120.02
124.13
124.31
124.55
125.02
125.45
125.73
127.71
128.12
128.93
129.01
129.43
129.54
145.35
145.98
146.09
151.53
151.91
154.14
172.44
ppm
20
40
60
80
100
120
140
160
180
ppm


S6B7>* dmso P non dec
-0.3477
2.9042
2.9837
3.6453
ppm
-10
-5
0
5
10
15
ppm

Sample Name	Formula	Adduct/Charge	Precursor Mass	Found At Mass	Mass Error (ppm)
Campione 7cB	C40H39BrClN6O6P	[M+H]+	845.1613	845.1593	-2.4 ppm



2. Cartesian Coordinates of optimized structures

6°

```
Stoichiometry    C25H17BrClN5O2
 Framework group  C1[X(C25H17BrClN5O2)]
 Deg. of freedom   147
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.966031    3.431296    0.783909
      2          6           0        1.299597    2.045108    0.682774
      3          6           0        1.911174    1.325831   -0.567257
      4          6           0        2.678111    2.446481   -1.314623
      5          6           0        3.096210    3.477983   -0.252709
      6          1           0        2.334866    3.696508    1.778852
      7          1           0        1.416221    1.421295    1.571539
      8          1           0        1.123766    0.911952   -1.200813
      9          1           0        3.521520    2.059878   -1.896029
     10          1           0        1.988178    2.925998   -2.018608
     11          1           0        3.194331    4.488352   -0.668841
     12          6           0       -0.152189    2.458646    0.468003
     13          8           0        0.925958    4.377859    0.418590
     14          7           0       -0.303268    3.723733    0.307615
     15          8           0        4.284928    3.108159    0.449857
     16          1           0        5.023016    3.111410   -0.179778
     17          6           0       -1.282138    1.500730    0.352225
     18          6           0       -1.666539    0.756796    1.489447
     19          6           0       -1.912034    1.284518   -0.894798
     20          6           0       -1.118409    1.025066    2.784505
     21          6           0       -2.657888   -0.290079    1.373832
     22          6           0       -2.916904    0.247824   -1.023360
     23          6           0       -1.586441    2.052627   -2.059490
     24          6           0       -1.479415    0.292074    3.883015
     25          1           0       -0.430812    1.856626    2.897349
     26          6           0       -2.997500   -1.037112    2.545618
     27          6           0       -3.239814   -0.512767    0.113663
     28          6           0       -3.525705    0.044577   -2.302120
     29          1           0       -0.865032    2.855135   -1.965893
     30          6           0       -2.196518    1.823028   -3.262944
     31          6           0       -2.423273   -0.762580    3.757599
     32          1           0       -1.054003    0.523602    4.855348
     33          1           0       -3.730406   -1.829678    2.458452
     34          6           0       -3.178372    0.803574   -3.386218
     35          1           0       -4.277246   -0.729086   -2.397953
     36          1           0       -1.935431    2.427780   -4.126861
     37          1           0       -2.700902   -1.344308    4.631788
     38          1           0       -3.658169    0.629004   -4.344979
     39         35           0       -4.541090   -1.915510   -0.058688
     40          6           0        2.484526   -1.122558   -0.669980
     41          6           0        3.815322    0.046680    0.633350
     42          6           0        3.468017   -1.929836   -0.056379
     43          1           0        4.222879    0.924392    1.116078
     44          6           0        3.394664   -3.283233   -0.396091
```


45	6	0	1.589288	-2.845440	-1.735009
46	1	0	0.842513	-3.255070	-2.409520
47	17	0	4.532665	-4.431233	0.266811
48	7	0	4.286923	-1.171676	0.753463
49	7	0	2.724284	0.157931	-0.215646
50	7	0	1.534363	-1.530747	-1.508310
51	7	0	2.466508	-3.731173	-1.224435

6a_up

Stoichiometry C25H17BrClN5O2
Framework group C1[X(C25H17BrClN5O2)]
Deg. of freedom 147
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.850097	2.994776	1.148476
2	6	0	1.138643	1.704523	0.714210
3	6	0	1.546584	1.431094	-0.777665
4	6	0	2.445946	2.630943	-1.189486
5	6	0	2.937535	3.327939	0.103495
6	1	0	2.272958	2.968707	2.157295
7	1	0	1.366242	0.836112	1.335284
8	1	0	0.651293	1.409576	-1.403151
9	1	0	3.284640	2.330216	-1.823106
10	1	0	1.831116	3.329580	-1.767085
11	1	0	2.987776	4.411718	-0.033351
12	6	0	-0.316399	2.138821	0.829279
13	8	0	0.799918	4.007743	1.131097
14	7	0	-0.449246	3.402611	1.020438
15	8	0	4.221014	2.932883	0.527054
16	1	0	4.233831	1.956034	0.623115
17	6	0	-1.471462	1.231609	0.606048
18	6	0	-1.719895	0.199582	1.537994
19	6	0	-2.257034	1.344353	-0.564586
20	6	0	-1.003817	0.118463	2.774906
21	6	0	-2.733876	-0.796858	1.271085
22	6	0	-3.281500	0.356906	-0.843488
23	6	0	-2.070035	2.405319	-1.510290
24	6	0	-1.234233	-0.889258	3.672486
25	1	0	-0.290911	0.900135	3.015291
26	6	0	-2.934428	-1.836988	2.232428
27	6	0	-3.471640	-0.686428	0.079334
28	6	0	-4.042290	0.487908	-2.048587
29	1	0	-1.339478	3.173434	-1.287011
30	6	0	-2.823726	2.490281	-2.650050
31	6	0	-2.205781	-1.887204	3.390290
32	1	0	-0.683378	-0.921034	4.608161
33	1	0	-3.686043	-2.589718	2.029216
34	6	0	-3.821364	1.516177	-2.924105
35	1	0	-4.807670	-0.249045	-2.257912
36	1	0	-2.666937	3.312084	-3.343078
37	1	0	-2.380368	-2.686679	4.104461
38	1	0	-4.415813	1.592305	-3.830027
39	35	0	-4.803348	-2.017965	-0.299471

40	6	0	3.248968	-0.468054	-0.397191
41	6	0	1.621664	-0.885128	-1.803301
42	6	0	3.321466	-1.779596	-0.923803
43	1	0	0.726647	-0.696653	-2.383469
44	6	0	4.390136	-2.543591	-0.448287
45	6	0	5.072249	-0.783861	0.847277
46	1	0	5.800411	-0.408464	1.560324
47	17	0	4.626105	-4.180019	-0.993036
48	7	0	2.288394	-2.011092	-1.804887
49	7	0	2.139699	0.101780	-0.979406
50	7	0	4.101206	0.062101	0.483505
51	7	0	5.249489	-2.046056	0.428083

6b

Stoichiometry C25H17BrClN5O2
Framework group C1[X(C25H17BrClN5O2)]
Deg. of freedom 147
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.653988	-0.327969	0.337904
2	6	0	1.676712	0.773202	0.644080
3	6	0	2.861151	0.152016	1.398468
4	6	0	2.193117	-0.988723	2.187823
5	6	0	0.996274	-1.484767	1.340733
6	1	0	0.707809	-0.709007	-0.683848
7	1	0	1.976292	1.383319	-0.216388
8	1	0	3.305785	0.901157	2.057224
9	1	0	2.886052	-1.798386	2.437917
10	1	0	1.817469	-0.568407	3.125466
11	1	0	0.141893	-1.719654	1.985739
12	7	0	-0.405685	1.453199	1.400671
13	8	0	1.321274	-2.629056	0.540811
14	1	0	1.466423	-3.383213	1.134665
15	6	0	-0.642548	0.439496	0.629705
16	8	0	0.970130	1.612018	1.592755
17	6	0	-2.035659	0.244903	0.149586
18	6	0	-2.819769	1.407703	-0.134555
19	6	0	-2.632353	-1.041963	0.016637
20	6	0	-2.255563	2.718008	-0.285558
21	6	0	-4.250340	1.288328	-0.343456
22	6	0	-4.065299	-1.163380	-0.176892
23	6	0	-1.885468	-2.261481	0.058245
24	6	0	-3.023522	3.817232	-0.560301
25	1	0	-1.187719	2.843096	-0.190488
26	6	0	-5.020381	2.469844	-0.589213
27	6	0	-4.826813	0.009413	-0.301661
28	6	0	-4.651118	-2.467827	-0.232358
29	1	0	-0.809549	-2.239238	0.092729
30	6	0	-2.483167	-3.491818	-0.030415
31	6	0	-4.430807	3.698624	-0.689328
32	1	0	-2.547601	4.785649	-0.685457
33	1	0	-6.090536	2.368010	-0.715254
34	6	0	-3.890264	-3.601400	-0.154188

35	1	0	-5.724018	-2.542690	-0.355781
36	1	0	-1.866981	-4.386827	-0.021248
37	1	0	-5.036223	4.578291	-0.888480
38	1	0	-4.360494	-4.578912	-0.209846
39	35	0	-6.737166	-0.144727	-0.457677
40	6	0	5.142410	0.425026	0.378894
41	6	0	4.035384	-1.316338	-0.385882
42	6	0	5.877872	-0.283968	-0.596294
43	1	0	3.222565	-2.025446	-0.475007
44	6	0	7.138554	0.254172	-0.869173
45	6	0	6.758859	1.910390	0.666561
46	1	0	7.151906	2.796557	1.157144
47	17	0	8.188890	-0.490495	-2.048997
48	7	0	3.950305	-0.257877	0.508030
49	7	0	5.161395	-1.368287	-1.056547
50	7	0	7.568833	1.337167	-0.244321
51	7	0	5.536277	1.516301	1.031863

6b_up

Stoichiometry C25H17BrClN5O2
Framework group C1[X(C25H17BrClN5O2)]
Deg. of freedom 147
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.853380	0.162422	0.808187
2	6	0	1.683877	1.424940	1.025277
3	6	0	2.963147	1.066458	1.795582
4	6	0	2.557470	-0.159633	2.634936
5	6	0	1.335453	-0.837547	1.943728
6	1	0	0.989116	-0.300388	-0.170888
7	1	0	1.872362	2.023696	0.123748
8	1	0	3.234756	1.912228	2.432208
9	1	0	3.370957	-0.878193	2.761964
10	1	0	2.270898	0.191202	3.630230
11	1	0	0.540291	-0.977738	2.680071
12	7	0	-0.487307	1.841677	1.711532
13	8	0	1.623286	-2.124630	1.448718
14	1	0	2.335482	-2.008552	0.782701
15	6	0	-0.544878	0.762360	1.000058
16	8	0	0.859542	2.190457	1.938325
17	6	0	-1.863222	0.377719	0.424540
18	6	0	-2.677363	1.409207	-0.137411
19	6	0	-2.340825	-0.961739	0.435876
20	6	0	-2.208041	2.746009	-0.366047
21	6	0	-4.034137	1.115177	-0.560384
22	6	0	-3.700364	-1.256671	0.025402
23	6	0	-1.534769	-2.068961	0.846134
24	6	0	-3.002020	3.715836	-0.915571
25	1	0	-1.193538	2.997480	-0.096685
26	6	0	-4.839312	2.168468	-1.100948
27	6	0	-4.505780	-0.199838	-0.426859
28	6	0	-4.170445	-2.605939	0.101158
29	1	0	-0.495194	-1.927428	1.088299

30	6	0	-2.017444	-3.350793	0.883321
31	6	0	-4.345388	3.431087	-1.271097
32	1	0	-2.596807	4.710000	-1.082158
33	1	0	-5.857043	1.939339	-1.389522
34	6	0	-3.360273	-3.624458	0.521727
35	1	0	-5.191600	-2.810535	-0.194181
36	1	0	-1.356854	-4.158442	1.185537
37	1	0	-4.974937	4.209915	-1.692064
38	1	0	-3.741509	-4.640784	0.564593
39	35	0	-6.330640	-0.576187	-0.907689
40	6	0	4.434955	-0.124038	0.019034
41	6	0	5.167066	1.789303	0.801050
42	6	0	5.658117	0.268175	-0.577315
43	1	0	5.173038	2.686668	1.407766
44	6	0	6.160776	-0.616427	-1.535141
45	6	0	4.366041	-1.993183	-1.201219
46	1	0	3.867367	-2.918878	-1.473886
47	17	0	7.654819	-0.277716	-2.359671
48	7	0	4.129231	0.877354	0.916704
49	7	0	6.092567	1.470222	-0.065894
50	7	0	5.515707	-1.731453	-1.840397
51	7	0	3.766225	-1.245814	-0.266894

6b'

Stoichiometry C25H17BrClN5O2
Framework group C1[X(C25H17BrClN5O2)]
Deg. of freedom 147
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432510	0.475719	-0.193405
2	6	0	-1.672896	0.208372	-1.071771
3	6	0	-2.599912	-0.767116	-0.299906
4	6	0	-1.688042	-1.377533	0.789596
5	6	0	-0.621299	-0.315354	1.123687
6	1	0	-0.268036	1.527065	0.057249
7	1	0	-2.205926	1.100648	-1.411132
8	1	0	-2.961337	-1.529780	-0.992565
9	1	0	-2.245629	-1.711338	1.670642
10	1	0	-1.191681	-2.258208	0.365827
11	1	0	0.317387	-0.776434	1.455887
12	7	0	0.232381	-0.572595	-2.190181
13	8	0	-1.061145	0.634970	2.097984
14	1	0	-1.164701	0.174831	2.946206
15	6	0	0.668176	-0.060897	-1.097142
16	8	0	-1.159000	-0.468962	-2.252899
17	6	0	2.113641	-0.039402	-0.747527
18	6	0	2.792697	1.198149	-0.728061
19	6	0	2.776302	-1.228259	-0.369608
20	6	0	2.175115	2.401539	-1.197005
21	6	0	4.156344	1.272808	-0.250465
22	6	0	4.143866	-1.171536	0.106999
23	6	0	2.137313	-2.508946	-0.433588
24	6	0	2.831182	3.602538	-1.168305

25	1	0	1.177306	2.344618	-1.618684
26	6	0	4.799732	2.550372	-0.229737
27	6	0	4.778068	0.081661	0.163240
28	6	0	4.776911	-2.392791	0.501273
29	1	0	1.132086	-2.564167	-0.833750
30	6	0	2.784287	-3.652252	-0.049325
31	6	0	4.158777	3.678177	-0.666983
32	1	0	2.342266	4.498483	-1.540023
33	1	0	5.817559	2.610254	0.135349
34	6	0	4.121168	-3.591794	0.429130
35	1	0	5.798354	-2.352349	0.858728
36	1	0	2.279168	-4.611509	-0.119351
37	1	0	4.672148	4.635079	-0.643799
38	1	0	4.627530	-4.503851	0.731908
39	35	0	6.579091	0.171298	0.827026
40	6	0	-5.094458	-0.476790	-0.184549
41	6	0	-3.980275	0.931591	1.085935
42	6	0	-5.952976	0.409006	0.503540
43	1	0	-3.119219	1.384463	1.558778
44	6	0	-7.311556	0.210774	0.242987
45	6	0	-6.785087	-1.510320	-1.172940
46	1	0	-7.161742	-2.276352	-1.845119
47	17	0	-8.520948	1.213437	1.007216
48	7	0	-3.817715	-0.127926	0.205365
49	7	0	-5.228771	1.279077	1.290539
50	7	0	-7.718015	-0.736819	-0.584728
51	7	0	-5.459856	-1.443119	-1.024112

6b'_up

Stoichiometry C25H17BrClN5O2
Framework group C1[X(C25H17BrClN5O2)]
Deg. of freedom 147
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.585898	-0.427057	0.480583
2	6	0	-1.753820	0.071701	1.348551
3	6	0	-2.448202	1.232197	0.566161
4	6	0	-1.646679	1.413409	-0.751215
5	6	0	-0.770849	0.150444	-0.955443
6	1	0	-0.509049	-1.515577	0.398700
7	1	0	-2.470790	-0.694263	1.651321
8	1	0	-2.376370	2.124926	1.191184
9	1	0	-2.290322	1.582831	-1.618427
10	1	0	-1.003563	2.293750	-0.646458
11	1	0	0.197480	0.419452	-1.386437
12	7	0	0.241725	0.674882	2.393484
13	8	0	-1.322179	-0.793020	-1.842787
14	1	0	-2.229414	-1.010493	-1.537762
15	6	0	0.583077	0.130697	1.282016
16	8	0	-1.150956	0.592035	2.558514
17	6	0	2.002203	0.076108	0.837540
18	6	0	2.669264	-1.167517	0.823090
19	6	0	2.645266	1.241494	0.365170

20	6	0	2.077377	-2.343834	1.384486
21	6	0	3.995515	-1.275263	0.254762
22	6	0	3.975884	1.152126	-0.202115
23	6	0	2.022656	2.530503	0.421706
24	6	0	2.721064	-3.551483	1.359962
25	1	0	1.111363	-2.259019	1.870329
26	6	0	4.625867	-2.559371	0.241263
27	6	0	4.595583	-0.108488	-0.250106
28	6	0	4.588673	2.350079	-0.689059
29	1	0	1.048085	2.611629	0.887548
30	6	0	2.649204	3.650945	-0.052782
31	6	0	4.008964	-3.661376	0.769377
32	1	0	2.252933	-4.426650	1.801455
33	1	0	5.614088	-2.645212	-0.193394
34	6	0	3.948680	3.557723	-0.620572
35	1	0	5.582015	2.284495	-1.115299
36	1	0	2.157352	4.617443	0.012856
37	1	0	4.511742	-4.623989	0.748580
38	1	0	4.439014	4.451562	-0.995475
39	35	0	6.345739	-0.243454	-1.032201
40	6	0	-4.552447	0.002395	-0.253245
41	6	0	-4.891568	1.832373	0.901716
42	6	0	-5.929925	0.276397	-0.081190
43	1	0	-4.638640	2.720734	1.467390
44	6	0	-6.789477	-0.659418	-0.662546
45	6	0	-4.984414	-1.853580	-1.409928
46	1	0	-4.634027	-2.723644	-1.957448
47	17	0	-8.516338	-0.475022	-0.545277
48	7	0	-3.890675	1.023280	0.389120
49	7	0	-6.111263	1.432096	0.645958
50	7	0	-6.315247	-1.709297	-1.315714
51	7	0	-4.043964	-1.045398	-0.906677

7cA

Stoichiometry C40H39BrClN6O6P
Framework group C1[X(C40H39BrClN6O6P)]
Deg. of freedom 276
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015775	-1.697915	0.506217
2	6	0	1.277892	-0.860449	0.538222
3	6	0	1.200245	0.161331	-0.647895
4	6	0	-0.001404	-0.324003	-1.498000
5	6	0	-0.942628	-1.073623	-0.548800
6	1	0	-0.521879	-1.809162	1.469043
7	1	0	1.452995	-0.334818	1.479212
8	1	0	2.119114	0.133892	-1.237502
9	1	0	-0.506286	0.483009	-2.032552
10	1	0	0.373010	-1.036356	-2.242237
11	1	0	-1.535797	-1.843813	-1.045879
12	6	0	2.312752	-1.954436	0.297379
13	8	0	0.398018	-3.015289	0.056015
14	7	0	1.793595	-3.094622	0.016310

15	8	0	-1.807729	-0.155139	0.154799
16	6	0	3.780658	-1.723946	0.278796
17	6	0	4.435332	-1.383855	1.482977
18	6	0	4.496265	-1.774779	-0.939401
19	6	0	3.759471	-1.423704	2.744372
20	6	0	5.832466	-1.009890	1.471136
21	6	0	5.899410	-1.412483	-0.965392
22	6	0	3.880601	-2.165492	-2.172608
23	6	0	4.391745	-1.080091	3.909056
24	1	0	2.733037	-1.773794	2.774897
25	6	0	6.450042	-0.649298	2.710097
26	6	0	6.511125	-1.027515	0.240093
27	6	0	6.591298	-1.457700	-2.216944
28	1	0	2.843115	-2.476108	-2.158193
29	6	0	4.583486	-2.195905	-3.346499
30	6	0	5.753451	-0.675065	3.888246
31	1	0	3.856789	-1.128190	4.853260
32	1	0	7.493016	-0.357852	2.701715
33	6	0	5.957281	-1.834645	-3.369281
34	1	0	7.639467	-1.186603	-2.236554
35	1	0	4.091801	-2.505183	-4.264553
36	1	0	6.247659	-0.398174	4.814932
37	1	0	6.507489	-1.862046	-4.305439
38	35	0	8.360819	-0.509149	0.207880
39	6	0	2.059326	2.517133	-0.518358
40	6	0	0.198375	2.199010	0.612071
41	6	0	1.630125	3.692470	0.136129
42	1	0	-0.665653	1.674873	0.996467
43	6	0	2.460711	4.798238	-0.064151
44	6	0	3.838358	3.521204	-1.373547
45	1	0	4.741689	3.491182	-1.976511
46	17	0	2.084980	6.339478	0.667395
47	7	0	0.464448	3.464008	0.835123
48	7	0	1.120051	1.556088	-0.203780
49	7	0	3.145369	2.383989	-1.276673
50	7	0	3.549439	4.709746	-0.809515
51	15	0	-3.368534	0.104101	-0.220357
52	8	0	-4.007873	-1.389126	-0.241547
53	6	0	-4.722204	-2.010529	0.789461
54	6	0	-4.558946	-1.674486	2.132950
55	6	0	-5.594431	-3.023231	0.390629
56	6	0	-5.295695	-2.375529	3.090822
57	1	0	-3.893964	-0.870442	2.425403
58	6	0	-6.317264	-3.714763	1.362221
59	1	0	-5.705119	-3.245227	-0.665712
60	6	0	-6.171223	-3.394806	2.714058
61	1	0	-5.178355	-2.116955	4.139436
62	1	0	-6.997852	-4.504564	1.056977
63	1	0	-6.736262	-3.935368	3.467713
64	8	0	-3.911358	1.108661	0.716966
65	7	0	-3.423455	0.466293	-1.863320
66	1	0	-3.504130	1.474563	-1.958041
67	6	0	-4.225107	-0.252720	-2.879081
68	6	0	-5.678197	-0.548250	-2.457343
69	8	0	-6.312567	-1.503552	-2.851600
70	8	0	-6.151342	0.407122	-1.646159
71	6	0	-7.492714	0.238272	-1.113581
72	1	0	-8.205238	0.554448	-1.885654
73	1	0	-7.650388	-0.825214	-0.918167

74	6	0	-7.621695	1.072210	0.160694
75	1	0	-6.829360	0.729898	0.840299
76	6	0	-9.001007	0.783223	0.816515
77	1	0	-9.469827	-0.085667	0.332726
78	1	0	-9.679414	1.625715	0.627189
79	6	0	-7.380090	2.567977	-0.124303
80	1	0	-6.427975	2.668182	-0.656705
81	1	0	-8.164143	2.929934	-0.807345
82	6	0	-8.925285	0.508405	2.323774
83	1	0	-8.490207	1.354864	2.865719
84	1	0	-9.921089	0.318504	2.741309
85	1	0	-8.301692	-0.369860	2.529381
86	6	0	-7.336154	3.452817	1.125538
87	1	0	-8.286343	3.443591	1.672009
88	1	0	-6.546223	3.120289	1.808856
89	1	0	-7.124535	4.493717	0.855475
90	1	0	-4.307394	0.451923	-3.717059
91	6	0	-3.535662	-1.515202	-3.397517
92	1	0	-2.549012	-1.261014	-3.795413
93	1	0	-3.422578	-2.255847	-2.601918
94	1	0	-4.136706	-1.966566	-4.190062

7cA_up

Stoichiometry C40H39BrClN6O6P
Framework group C1[X(C40H39BrClN6O6P)]
Deg. of freedom 276
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.697482	-2.342126	0.337824
2	6	0	1.681731	-1.159798	0.397142
3	6	0	1.256766	-0.146820	-0.726007
4	6	0	0.242514	-0.940357	-1.574285
5	6	0	-0.426319	-1.939404	-0.624482
6	1	0	0.305933	-2.665025	1.305896
7	1	0	1.713435	-0.667624	1.370255
8	1	0	2.123841	0.122610	-1.336727
9	1	0	-0.465144	-0.317644	-2.117181
10	1	0	0.818021	-1.516469	-2.307940
11	1	0	-0.845174	-2.804179	-1.143115
12	6	0	2.985616	-1.874936	0.065421
13	8	0	1.463686	-3.437284	-0.233863
14	7	0	2.816358	-3.096209	-0.295618
15	8	0	-1.433578	-1.304011	0.188662
16	6	0	4.315350	-1.212035	0.045984
17	6	0	4.863625	-0.744120	1.261819
18	6	0	4.985587	-0.983541	-1.178689
19	6	0	4.260000	-1.045356	2.525413
20	6	0	6.080565	0.038858	1.259346
21	6	0	6.213010	-0.212004	-1.194901
22	6	0	4.487312	-1.479458	-2.427334
23	6	0	4.781301	-0.574370	3.700742
24	1	0	3.393074	-1.697105	2.547664
25	6	0	6.584617	0.516467	2.510166

26	6	0	6.706708	0.284090	0.024466
27	6	0	6.857512	0.015783	-2.451971
28	1	0	3.593675	-2.091096	-2.421992
29	6	0	5.139408	-1.236878	-3.606164
30	6	0	5.953255	0.228878	3.690290
31	1	0	4.306818	-0.825631	4.644928
32	1	0	7.488751	1.112548	2.508704
33	6	0	6.339986	-0.477255	-3.618713
34	1	0	7.774589	0.591345	-2.464222
35	1	0	4.742895	-1.634588	-4.536056
36	1	0	6.357999	0.603809	4.625722
37	1	0	6.851468	-0.291072	-4.558639
38	35	0	8.310259	1.339782	0.005598
39	6	0	-0.367947	1.888409	-0.370829
40	6	0	1.557087	1.896154	0.689820
41	6	0	-0.165636	3.071460	0.386184
42	1	0	2.529661	1.539969	1.006210
43	6	0	-1.193259	4.013767	0.317454
44	6	0	-2.347692	2.637264	-1.089237
45	1	0	-3.256671	2.484236	-1.662709
46	17	0	-1.079882	5.515080	1.193497
47	7	0	1.045680	3.047251	1.037383
48	7	0	0.764476	1.124527	-0.148385
49	7	0	-1.448371	1.648480	-1.123030
50	7	0	-2.273100	3.795825	-0.414276
51	15	0	-3.022472	-1.500767	-0.078406
52	8	0	-3.226624	-3.094935	-0.348186
53	6	0	-3.719532	-3.972609	0.629055
54	6	0	-2.868358	-4.971305	1.095759
55	6	0	-5.046678	-3.887233	1.046071
56	6	0	-3.357832	-5.905382	2.010529
57	1	0	-1.845056	-5.017303	0.735509
58	6	0	-5.519225	-4.825728	1.964092
59	1	0	-5.686376	-3.101840	0.658365
60	6	0	-4.681370	-5.833341	2.447939
61	1	0	-2.701414	-6.689369	2.378033
62	1	0	-6.551204	-4.767749	2.298707
63	1	0	-5.059629	-6.561063	3.160338
64	8	0	-3.823090	-0.936388	1.029461
65	7	0	-3.169425	-0.906368	-1.639978
66	1	0	-2.675686	-0.012664	-1.685477
67	6	0	-4.453275	-0.901353	-2.384480
68	6	0	-5.620059	-0.464884	-1.480632
69	8	0	-6.511291	-1.198662	-1.108874
70	8	0	-5.501397	0.826733	-1.131596
71	6	0	-6.405241	1.284758	-0.088207
72	1	0	-7.435299	1.105962	-0.416070
73	1	0	-6.210479	0.672913	0.797082
74	6	0	-6.144978	2.764295	0.185836
75	1	0	-5.083600	2.860285	0.454728
76	6	0	-7.000529	3.203812	1.407778
77	1	0	-7.419214	2.316935	1.903690
78	1	0	-7.866378	3.780949	1.056599
79	6	0	-6.402219	3.621248	-1.070255
80	1	0	-5.861638	3.177437	-1.915846
81	1	0	-7.470775	3.556899	-1.326083
82	6	0	-6.226958	4.015907	2.454220
83	1	0	-5.800144	4.929108	2.025842
84	1	0	-6.878078	4.307709	3.286617

85	1	0	-5.398829	3.428716	2.868310
86	6	0	-5.990116	5.091155	-0.934037
87	1	0	-6.561412	5.604710	-0.152433
88	1	0	-4.925367	5.178251	-0.687983
89	1	0	-6.163683	5.631033	-1.872325
90	1	0	-4.335230	-0.127709	-3.151065
91	6	0	-4.739498	-2.239532	-3.060704
92	1	0	-3.893929	-2.516501	-3.696604
93	1	0	-4.900690	-3.028131	-2.324325
94	1	0	-5.640281	-2.162952	-3.677736

7cB

Stoichiometry C40H39BrClN6O6P
Framework group C1[X(C40H39BrClN6O6P)]
Deg. of freedom 276
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.289188	-2.339505	-0.506420
2	6	0	-1.461024	-3.341159	-0.411071
3	6	0	-2.495785	-2.770670	0.592517
4	6	0	-1.722754	-1.679641	1.366949
5	6	0	-0.635066	-1.144052	0.421382
6	1	0	-0.092812	-1.960242	-1.512852
7	1	0	-1.918046	-3.614955	-1.365738
8	1	0	-2.813677	-3.576515	1.257115
9	1	0	-2.361362	-0.881838	1.750168
10	1	0	-1.232221	-2.155987	2.223838
11	1	0	0.242098	-0.771558	0.955763
12	7	0	0.494381	-4.390049	0.340324
13	8	0	-1.147079	-0.097610	-0.433158
14	6	0	-4.972760	-2.876295	0.218675
15	6	0	-3.969057	-1.350733	-1.009551
16	6	0	-5.879350	-2.190736	-0.618968
17	1	0	-3.162492	-0.738704	-1.389382
18	6	0	-7.206173	-2.612420	-0.496697
19	6	0	-6.570016	-4.143109	1.083333
20	1	0	-6.889274	-4.930354	1.760738
21	17	0	-8.467395	-1.876303	-1.455006
22	7	0	-5.224190	-1.243473	-1.375697
23	7	0	-3.736966	-2.320371	-0.042699
24	7	0	-5.267451	-3.849384	1.078129
25	7	0	-7.542787	-3.575967	0.344190
26	15	0	-1.130320	1.495646	-0.102451
27	8	0	0.427505	1.823814	0.211170
28	6	0	1.453665	1.917877	-0.742240
29	6	0	1.248146	2.477425	-2.003498
30	6	0	2.710282	1.476519	-0.334845
31	6	0	2.339060	2.579683	-2.869817
32	1	0	0.260576	2.814926	-2.295684
33	6	0	3.789199	1.589678	-1.211518
34	1	0	2.834432	1.054922	0.657202
35	6	0	3.605597	2.140202	-2.481539
36	1	0	2.190131	3.009700	-3.856512

37	1	0	4.761528	1.217953	-0.903151
38	1	0	4.445496	2.223890	-3.165117
39	8	0	-1.815140	2.199749	-1.207429
40	7	0	-1.796423	1.732085	1.425351
41	1	0	-2.696405	2.182308	1.281972
42	6	0	-1.101079	2.286530	2.608338
43	6	0	-0.397513	3.634715	2.358135
44	8	0	0.571484	4.018559	2.974507
45	8	0	-1.038730	4.347618	1.418891
46	6	0	-0.457065	5.624323	1.052295
47	1	0	-0.464871	6.279293	1.931649
48	1	0	0.585883	5.451841	0.769847
49	6	0	-1.266561	6.205188	-0.106510
50	1	0	-1.272187	5.441308	-0.897535
51	6	0	-0.550660	7.476197	-0.641503
52	1	0	0.475898	7.515935	-0.250684
53	1	0	-1.050927	8.369778	-0.244617
54	6	0	-2.726761	6.461367	0.319443
55	1	0	-3.127086	5.538205	0.754673
56	1	0	-2.730195	7.210740	1.125685
57	6	0	-0.480677	7.558522	-2.171612
58	1	0	-1.476766	7.543620	-2.626068
59	1	0	0.021080	8.478319	-2.493796
60	1	0	0.081084	6.710927	-2.582191
61	6	0	-3.657369	6.921169	-0.807618
62	1	0	-3.353767	7.889154	-1.221683
63	1	0	-3.674185	6.194194	-1.628308
64	1	0	-4.684184	7.030469	-0.440516
65	1	0	-1.908501	2.513491	3.317546
66	6	0	-0.160397	1.291357	3.286659
67	1	0	-0.710805	0.387804	3.563757
68	1	0	0.672248	1.021262	2.633370
69	1	0	0.260305	1.743680	4.187425
70	8	0	-0.879012	-4.549387	0.156603
71	6	0	0.858070	-3.212491	-0.015334
72	6	0	2.277910	-2.769925	0.038844
73	6	0	2.852270	-2.354477	1.258825
74	6	0	3.015584	-2.706663	-1.162605
75	6	0	2.158236	-2.477629	2.505779
76	6	0	4.180387	-1.775236	1.271153
77	6	0	4.348503	-2.144833	-1.166928
78	6	0	2.486026	-3.199776	-2.397547
79	6	0	2.711759	-2.041280	3.679476
80	1	0	1.189405	-2.963921	2.510782
81	6	0	4.712943	-1.322511	2.519976
82	6	0	4.871052	-1.678716	0.051234
83	6	0	5.059012	-2.088388	-2.406759
84	1	0	1.507516	-3.668074	-2.394223
85	6	0	3.202933	-3.130894	-3.561606
86	6	0	4.003316	-1.447167	3.683947
87	1	0	2.168562	-2.157559	4.612957
88	1	0	5.700887	-0.878681	2.529119
89	6	0	4.505182	-2.561517	-3.565629
90	1	0	6.056011	-1.665646	-2.410744
91	1	0	2.781795	-3.521336	-4.483547
92	1	0	4.433033	-1.098510	4.618498
93	1	0	5.067773	-2.511106	-4.493371
94	35	0	6.600203	-0.838962	0.039164

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Stoichiometry C40H39BrClN6O6P
Framework group C1[X(C40H39BrClN6O6P)]
Deg. of freedom 276
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.010849	-2.344846	-0.214053
2	6	0	0.280625	-3.681151	0.018152
3	6	0	-0.868415	-3.433787	1.032644
4	6	0	-0.454492	-2.125498	1.730920
5	6	0	0.336173	-1.292242	0.707268
6	1	0	0.970818	-1.982585	-1.243487
7	1	0	-0.055081	-4.170867	-0.899754
8	1	0	-0.880448	-4.260709	1.748680
9	1	0	-1.276317	-1.575159	2.183328
10	1	0	0.235110	-2.409584	2.534413
11	1	0	1.062424	-0.635846	1.192373
12	7	0	2.517035	-3.926561	0.662113
13	8	0	-0.526496	-0.501535	-0.134720
14	6	0	-3.287250	-2.605214	0.417303
15	6	0	-2.617510	-4.542681	-0.372750
16	6	0	-4.296000	-3.269887	-0.326363
17	1	0	-1.956507	-5.383233	-0.541494
18	6	0	-5.520516	-2.604668	-0.410858
19	6	0	-4.674357	-0.909132	0.860393
20	1	0	-4.854001	0.060148	1.314247
21	17	0	-6.849873	-3.302221	-1.293556
22	7	0	-3.847730	-4.478744	-0.806347
23	7	0	-2.187566	-3.444016	0.360390
24	7	0	-3.452724	-1.427131	1.027549
25	7	0	-5.704729	-1.435205	0.178487
26	15	0	-0.858304	1.067581	0.123188
27	8	0	0.545135	1.745394	0.588482
28	6	0	1.337661	2.604511	-0.186195
29	6	0	0.810860	3.744263	-0.792403
30	6	0	2.699134	2.318042	-0.232050
31	6	0	1.683280	4.595790	-1.473342
32	1	0	-0.249916	3.956343	-0.731258
33	6	0	3.560072	3.183594	-0.906996
34	1	0	3.072492	1.432787	0.270538
35	6	0	3.051826	4.322747	-1.533673
36	1	0	1.284356	5.485430	-1.952917
37	1	0	4.621723	2.955860	-0.930160
38	1	0	3.719556	4.997832	-2.061625
39	8	0	-1.502772	1.670659	-1.063886
40	7	0	-1.662074	1.007303	1.593788
41	1	0	-2.345520	0.247471	1.558481
42	6	0	-2.174477	2.219090	2.279401
43	6	0	-2.905904	3.152508	1.297576
44	8	0	-2.504406	4.244502	0.958317
45	8	0	-4.037863	2.582640	0.846932
46	6	0	-4.701879	3.266400	-0.250760
47	1	0	-4.862720	4.311575	0.034796

48	1	0	-4.018769	3.241240	-1.104898
49	6	0	-6.017731	2.553151	-0.559890
50	1	0	-5.773548	1.504498	-0.781969
51	6	0	-6.642833	3.187534	-1.832984
52	1	0	-5.879793	3.775599	-2.361710
53	1	0	-7.418057	3.907406	-1.536779
54	6	0	-6.959407	2.581806	0.661672
55	1	0	-6.398696	2.244829	1.542578
56	1	0	-7.239176	3.626972	0.862999
57	6	0	-7.228591	2.171542	-2.822314
58	1	0	-8.014593	1.562077	-2.364880
59	1	0	-7.660463	2.677287	-3.693837
60	1	0	-6.451355	1.488340	-3.184523
61	6	0	-8.223470	1.725636	0.524526
62	1	0	-8.874586	2.082326	-0.281194
63	1	0	-7.968072	0.679986	0.315770
64	1	0	-8.808960	1.749747	1.451098
65	1	0	-2.924865	1.848509	2.986613
66	6	0	-1.086174	2.963867	3.048285
67	1	0	-0.578979	2.272911	3.727338
68	1	0	-0.349608	3.400102	2.372131
69	1	0	-1.530574	3.776678	3.631220
70	8	0	1.261242	-4.547110	0.648946
71	6	0	2.426498	-2.737421	0.188310
72	6	0	3.611400	-1.847119	0.062184
73	6	0	4.191899	-1.255531	1.205589
74	6	0	4.107213	-1.559696	-1.228563
75	6	0	3.756235	-1.572365	2.532814
76	6	0	5.255969	-0.283123	1.051468
77	6	0	5.166806	-0.590177	-1.399873
78	6	0	3.603139	-2.219047	-2.394871
79	6	0	4.312778	-0.973646	3.630493
80	1	0	2.991234	-2.329333	2.658629
81	6	0	5.799189	0.323962	2.227725
82	6	0	5.688784	0.025912	-0.249690
83	6	0	5.625146	-0.308332	-2.725049
84	1	0	2.853276	-2.993407	-2.273843
85	6	0	4.076990	-1.926017	-3.645217
86	6	0	5.344564	-0.008502	3.474839
87	1	0	3.969488	-1.239749	4.626159
88	1	0	6.585520	1.059380	2.111252
89	6	0	5.095381	-0.949144	-3.812159
90	1	0	6.411100	0.425443	-2.853470
91	1	0	3.681782	-2.447257	-4.512323
92	1	0	5.776551	0.465238	4.351543
93	1	0	5.462717	-0.718417	-4.807826
94	35	0	7.041139	1.371471	-0.473346

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Stoichiometry C40H39BrClN6O6P
Framework group C1[X(C40H39BrClN6O6P)]
Deg. of freedom 276
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.598124	-2.280471	0.391770
2	6	0	1.935903	-3.045523	0.361891
3	6	0	2.820450	-2.421422	-0.749043
4	6	0	1.832635	-1.628106	-1.634045
5	6	0	0.630155	-1.236032	-0.755541
6	1	0	0.392622	-1.767490	1.333349
7	1	0	2.460527	-3.099339	1.320013
8	1	0	3.301148	-3.229837	-1.303626
9	1	0	2.283086	-0.758171	-2.117858
10	1	0	1.475247	-2.296436	-2.425014
11	1	0	-0.294134	-1.224343	-1.335970
12	7	0	0.195180	-4.545061	-0.090308
13	8	0	0.826375	0.082641	-0.179891
14	6	0	5.243081	-2.062810	-0.181107
15	6	0	3.937220	-0.398967	0.420507
16	6	0	5.960246	-1.035468	0.471393
17	1	0	3.026586	0.174705	0.519425
18	6	0	7.330358	-1.280469	0.593391
19	6	0	7.064173	-3.287202	-0.476847
20	1	0	7.548794	-4.186049	-0.847860
21	17	0	8.377555	-0.117962	1.372875
22	7	0	5.118108	-0.007328	0.836659
23	7	0	3.931843	-1.633801	-0.209029
24	7	0	5.745805	-3.195352	-0.667502
25	7	0	7.871278	-2.392240	0.125388
26	15	0	-0.181971	1.294312	-0.596086
27	8	0	0.770473	2.558460	-0.244990
28	6	0	2.020954	2.794191	-0.830513
29	6	0	2.214519	2.682222	-2.207594
30	6	0	3.043749	3.199080	0.023934
31	6	0	3.480192	2.964218	-2.727071
32	1	0	1.389806	2.389735	-2.848894
33	6	0	4.300828	3.478522	-0.513107
34	1	0	2.842804	3.292287	1.086556
35	6	0	4.522936	3.358998	-1.886706
36	1	0	3.645155	2.879521	-3.797766
37	1	0	5.107674	3.780249	0.147727
38	1	0	5.504211	3.573495	-2.299697
39	8	0	-0.736214	1.176099	-1.964530
40	7	0	-1.368766	1.395103	0.569317
41	1	0	-2.239641	1.687290	0.137427
42	6	0	-1.197296	1.923932	1.935606
43	6	0	-0.849841	3.425069	1.959887
44	8	0	-0.046806	3.934480	2.709551
45	8	0	-1.599799	4.102849	1.072267
46	6	0	-1.343023	5.525561	0.970900
47	1	0	-1.508185	5.982931	1.953418
48	1	0	-0.288867	5.660731	0.710030
49	6	0	-2.263954	6.119505	-0.094460
50	1	0	-2.063450	5.575452	-1.029449
51	6	0	-1.890834	7.612787	-0.304398
52	1	0	-0.901604	7.809685	0.131901
53	1	0	-2.591594	8.244354	0.258210
54	6	0	-3.744917	5.905432	0.280101
55	1	0	-3.899368	4.839555	0.485583
56	1	0	-3.945580	6.432302	1.225251
57	6	0	-1.857605	8.054662	-1.772977
58	1	0	-2.824145	7.908158	-2.266143

59	1	0	-1.596656	9.115851	-1.857648
60	1	0	-1.110308	7.482454	-2.335725
61	6	0	-4.756626	6.358977	-0.777766
62	1	0	-4.713526	7.439720	-0.951923
63	1	0	-4.580921	5.858037	-1.737624
64	1	0	-5.778447	6.119807	-0.461888
65	1	0	-2.189169	1.840170	2.398765
66	6	0	-0.211688	1.112739	2.772980
67	1	0	-0.539166	0.070212	2.818142
68	1	0	0.798128	1.156206	2.357634
69	1	0	-0.169424	1.520447	3.785464
70	8	0	1.582056	-4.404385	-0.020148
71	6	0	-0.379457	-3.421989	0.146296
72	6	0	-1.855564	-3.253657	0.104341
73	6	0	-2.548857	-3.325487	-1.125122
74	6	0	-2.542043	-2.943583	1.298596
75	6	0	-1.896394	-3.685555	-2.348529
76	6	0	-3.964347	-3.016498	-1.173332
77	6	0	-3.951918	-2.622518	1.265564
78	6	0	-1.884548	-2.961828	2.570578
79	6	0	-2.577252	-3.737037	-3.534545
80	1	0	-0.847345	-3.953309	-2.316783
81	6	0	-4.632436	-3.082958	-2.436732
82	6	0	-4.609108	-2.659043	0.023352
83	6	0	-4.602453	-2.291442	2.496148
84	1	0	-0.847017	-3.275610	2.615781
85	6	0	-2.547775	-2.646548	3.726675
86	6	0	-3.963672	-3.429541	-3.579013
87	1	0	-2.058227	-4.020792	-4.445596
88	1	0	-5.689982	-2.853155	-2.474171
89	6	0	-3.924170	-2.294756	3.685334
90	1	0	-5.656516	-2.043655	2.472362
91	1	0	-2.027213	-2.681719	4.679511
92	1	0	-4.495891	-3.473427	-4.524835
93	1	0	-4.444311	-2.044395	4.605482
94	35	0	-6.475007	-2.202493	-0.038162