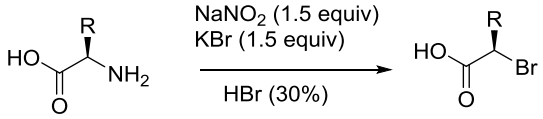
Supporting Information for

Solid Phase Synthesis of 1,3,4-oxadiazin-5 (6R)-one and 1,3,4-oxadiazol-2-one Scaffolds from Acyl Hydrazides

Synthesis of chiral 2-substituted-2-bromoacetic acids:



3, R = CH_2-$CH(CH_3)_2$; **4**, R = $CH(CH_3)_2$; **5**, R = CH_2-(CO)-Oallyl

Fig. S1. General route for the synthesis of chiral 2-substituted-2-bromoacetic acids.

Amino acid (1.0 eq) and KBr (1.5 eq) was dissolved in 100 ml, of a 30% HBr water solution and kept in −15°C dry ice/ethylene glycol bath. $NaNO_2$ (1.5 eq) were dissolved in minimum water and slowly dripped in the above solution under argon atmosphere. The reaction was allowed to proceed for 3 hr and to warm from −15°C to room temperature. It was then put under vacuum for 30 min. Product was extracted by diethyl ether. Organic phases were combined and dried over Na_2SO_4. Then the solvent was evaporated under vacuum. The product was characterized by NMR. No further purification needed.

3, ^{1}H-NMR (400 MHz; $CDCl_3$): δ 10.62 (br, 1H), 4.29 (t, *J* = 7.7 Hz, 1H), 1.94-1.90 (m, 2H), 1.86-1.76 (m, 1H), 0.98-0.92 (m, 6H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 176.4, 44.1, 43.3, 26.4, 22.5, 21.69, 21.55. $[\alpha]_D^{25}$ = − 34.2 (c = 1, MeOH)

4, ^{1}H-NMR (400 MHz; $CDCl_3$): δ 4.08 (d, *J* = 7.7 Hz, 1H), 2.31-2.19 (m, 1H), 1.10 (dd, *J* = 15.5, 6.7 Hz, 6H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 175.5, 54.1, 32.3, 20.2, 19.9. $[\alpha]_D^{25}$ = − 29.9 (c = 1, MeOH).

5, ^{1}H-NMR (400 MHz; $CDCl_3$): δ 5.90 (ddt, *J* = 17.2, 10.4, 5.8 Hz, 1H), 5.36-5.25 (m, 2H), 4.64-4.61 (m, 3H), 3.30 (dd, *J* = 17.3, 8.9 Hz, 1H), 3.04 (dd, *J* = 17.3, 6.1 Hz, 1H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 177.7, 169.4, 131.5, 119.1, 66.2, 46.3, 39.7.

$[\alpha]_D^{25}$ = − 15.2 (c = 1, MeOH)

Submonomer Synthesis :

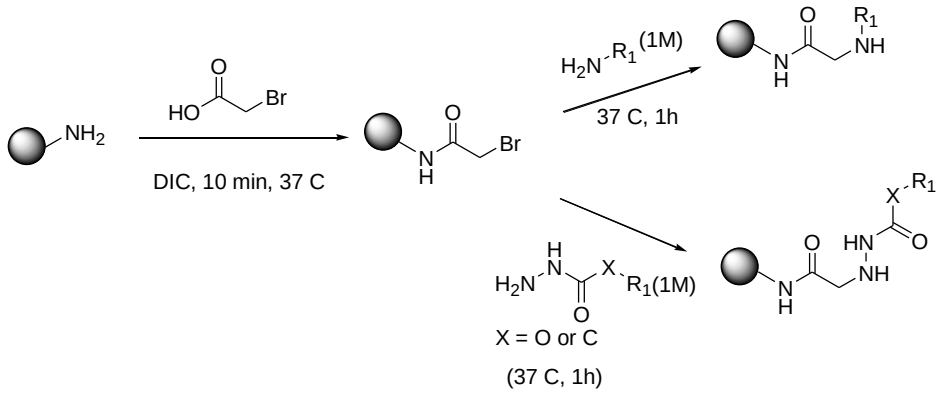


Fig. S2. Submonomer synthesis involving primary amines and acyl hydrazides.

Bromo acylation:

For bromo acylation, 100mg beads were treated with 1mL bromoacetic acid (2M) and 1mL diisopropylcarbodiimide (DIC) (3.8M) at 37 C for 10 mins.

SN2 displacement of resin-bound bromide:

100 mg of bromoacylated beads were treated with 2mL solution [1M in N-methylpyrrolidinone (NMP) or dimethylformamide (DMF)] of nucleophile (amine or acyl hydrazide or carbazate) for 1h at 37 °C to displace the bromide moiety.

Compound Cleavage from resin:

Resin-bound compounds were extensively washed with DCM. The DCM was drained and the compounds were cleaved from the resin by treating with 2 mL TFA cocktail [95% TFA, 2.5% trisisopropylsilane (TIPS) and 2.5% water] for 1h.

Solvent system for HPLC purification:

For HPLC purification a gradient of acetonitrile/water (0.1% TFA) was used.

Sample Preparation for MALDI:

α-Cyano-4-hydroxycinnamic acid matrix solution was prepared in a solution of 50% acetonitrile in water with 0.1% TFA. 1μL of compound solution obtained from an analytical HPLC run was taken and mixed with 1μL of matrix solution and spotted to MALDI plate to collect MALDI TOF MS spectra.

Oxadiazin-5(6R)-one ring formation:

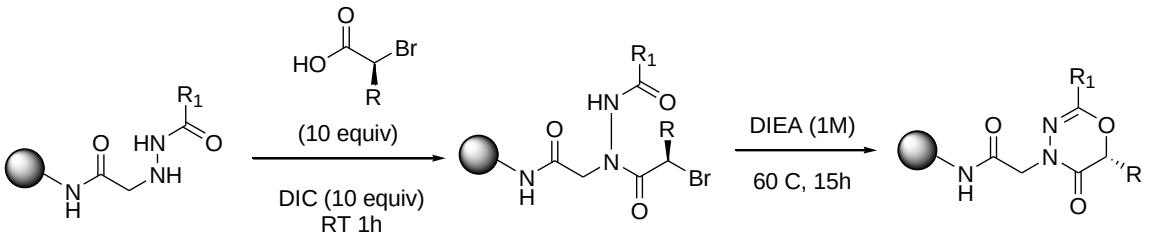


Fig. S3. When azapeptoids are N-bromoacylated with chiral 2-bromo acids and then treated with DIEA, 6-membered 1,3,4-oxadiazin-5(6R)-one are formed having a substituent and a chiral centre at the 6-position of the heterocycle.

100 mg of acyl hydrazide conjugated beads were washed with DMF and the beads were then treated with 10 equiv. of 2-substituted-2-bromoacetic acid (**1**-**5)** and 10 equiv. of diisopropylcarbodiimide (DIC) (overall volume 2mL DMF per 100mg beads) at 37 °C for 1h. The beads were then washed with DMF and incubated with 1M DIEA solution in N-methylpyrrolidione (NMP) at 60 °C for 15h (2mL for 100mg beads). The beads were then washed with DMF (5 times) followeds by DCM (5 times) and then incubated with DCM for 10 mins. The DCM was drained and the compounds were cleaved from the resin by treating with 2 mL TFA cocktail [95% TFA, 2.5% trisisopropylsilane (TIPS) and 2.5% water] for 1h.

Oxadiazol-2-one ring formation:

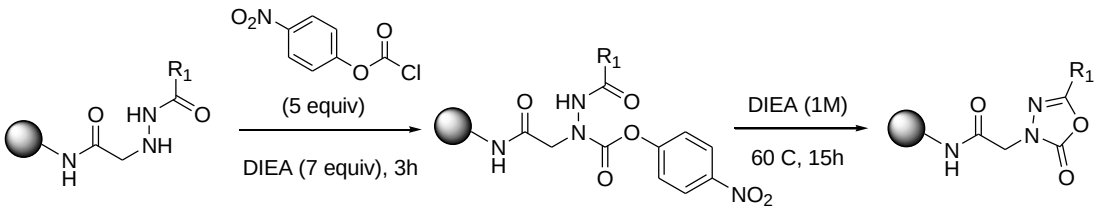


Fig. S4. When azapeptoids are N-acylated with 4-nitrophenyl chloroformate and then treated with 1M DIEA, 5-membered 1,3,4-oxadiazol-2-one are formed.

Acyl hydrazide conjugated beads were washed with DMF and dichloromethane (DCM) and incubated in DCM for 10 mins. DCM were drained and the beads were then treated with 5 equiv. of *p*-nitrophenyl chloroformate (in 2mL anhydrous DCM) and 7 equiv. of

diisopropylethylamine (DIEA) (in 2mL DCM) (overall volume 2mL per 100mg beads) at room temperature for 3h. The beads were then washed with DCM and DMF and incubated with 1M DIEA solution in N-methylpyrrolidione (NMP) at 60 C for 15h (2mL for 100mg beads). The beads were then washed with DMF (5 times) followed by DCM (5 times) and then incubated with DCM for 10 mins. The DCM was drained and the compounds were cleaved from the resin by treating with 4mL TFA cocktail [95% TFA, 2.5% trisisopropylsilane (TIPS) and 2.5% water] for 1h.

General Procedure for synthesis of compounds 6-13

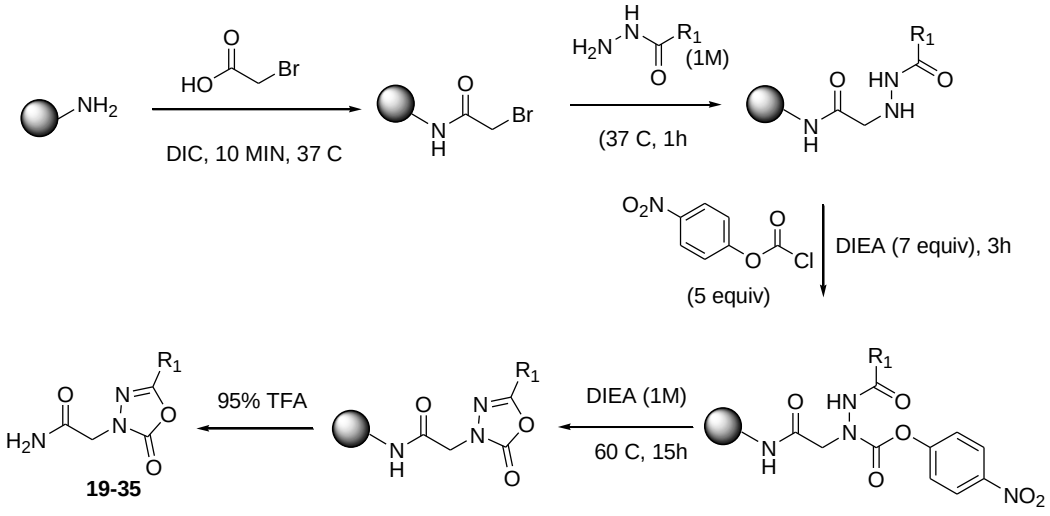
The compounds **6-13** were synthesized on knorr amide MBHA resin (Novabiochem, 0.75 mmol/g). The peptoid sequence (Nbsa-Nmea-Nmea) [Nbsa = 4-(2-aminoethyl)benzenesulfonamide; Nmea = 2-methoxyethylamine] was synthesized on the solid support using the sub-monomer synthesis method described above. The acylation step was carried out using bromoacetic acid in presence of DIC at 37 °C for 10 minutes and the bromide displacement was achieved by treating the beads with 1M solution of amines in NMP or DMF at 37 °C as described above. The resin-bound peptoid trimer (Nbsa-Nmea-Nmea) was washed with DMF and then acylated with bromoacetic acid in presence of DIC for 10 minutes at 37 °C following the protocol discussed above. The beads were washed with DMF and the terminal bromide was then displaced with different aryl and hetero-aromatic acyl hydrazides (1M in DMF or NMP) at 37 °C for 1h. The resin-bound acyl hydrazides were then washed with DMF and treated with different chiral 2-substituted-2-bromoacetic acids (**1**-**5**) (10 equiv.) in the presence of diisopropylcarbodiimide (DIC) (10 equiv.) in DMF at 37 °C for 1h. The beads were washed with DMF and then treated with a 1M DIEA solution in N-methylpyrrolidinone (NMP) for ~15 hours at 60 °C, which led to efficient formation of the 6-membered oxadiazinone ring-containing compounds **6-13** as evidenced by their HPLC traces and mass spectra.

General Procedure for synthesis of compounds 14-18

The compounds **14-18** were synthesized on knorr amide MBHA resin (Novabiochem, 0.75 mmol/g). The peptoid sequence (Nbsa-Nmea-Nmea) [Nbsa = 4-(2-

aminoethyl)benzenesulfonamide; Nmea = 2-methoxyethylamine] was synthesized on the solid support using the sub-monomer synthesis method described above. The acylation step was carried out using bromoacetic acid in presence of DIC at 37 °C for 10 minutes and the bromide displacement was achieved by treating the beads with 1M solution of amines in NMP or DMF at 37 °C as described above. The resin-bound peptoid trimer (Nbsa-Nmea-Nmea) was washed with DMF and then acylated with bromoacetic acid in presence of DIC for 10 minutes at 37 °C following the protocol discussed above. The beads were washed with DMF and the terminal bromide was then displaced with different aryl and hetero-aromatic acyl hydrazides (1M in DMF or NMP) at 37 °C for 1h. The beads were washed with DMF followed by DCM and incubated in DCM for 10 minutes. The acyl hydrazide-bound resin was then treated with 4-nitrophenyl chloroformate (5 equiv.) in the presence of DIEA (7 equiv.) in dichloromethane (DCM) at room temperature for 3 hours. The beads were washed with DMF and DCM and then treated with 1M DIEA in NMP for ~15 hours at 60 °C, which resulted in the highly efficient formation of the 5-membered oxadiazolone ring-containing compounds (**14-18**) (purity >95% from HPLC analysis).

General procedure for synthesis of compounds 19-35:



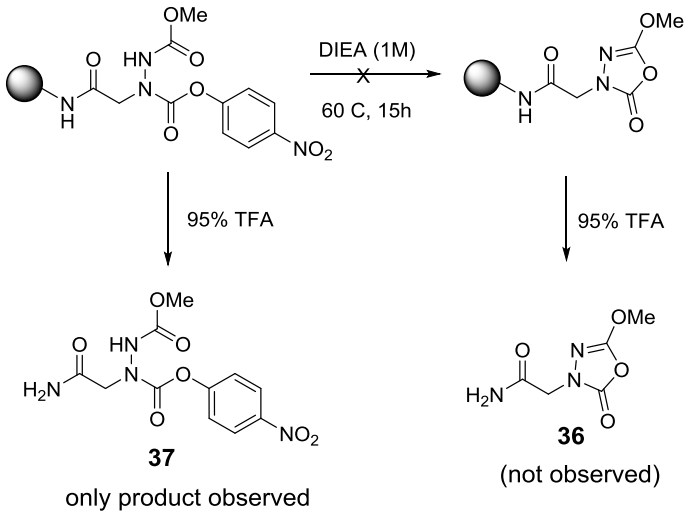


Fig. S5. General route for the synthesis of compounds **19**-**35**. Attempt to synthesize compound **36** having a methoxy group in the oxadiazolone ring failed under these conditions. The only product observed from this reaction was compound **37**.

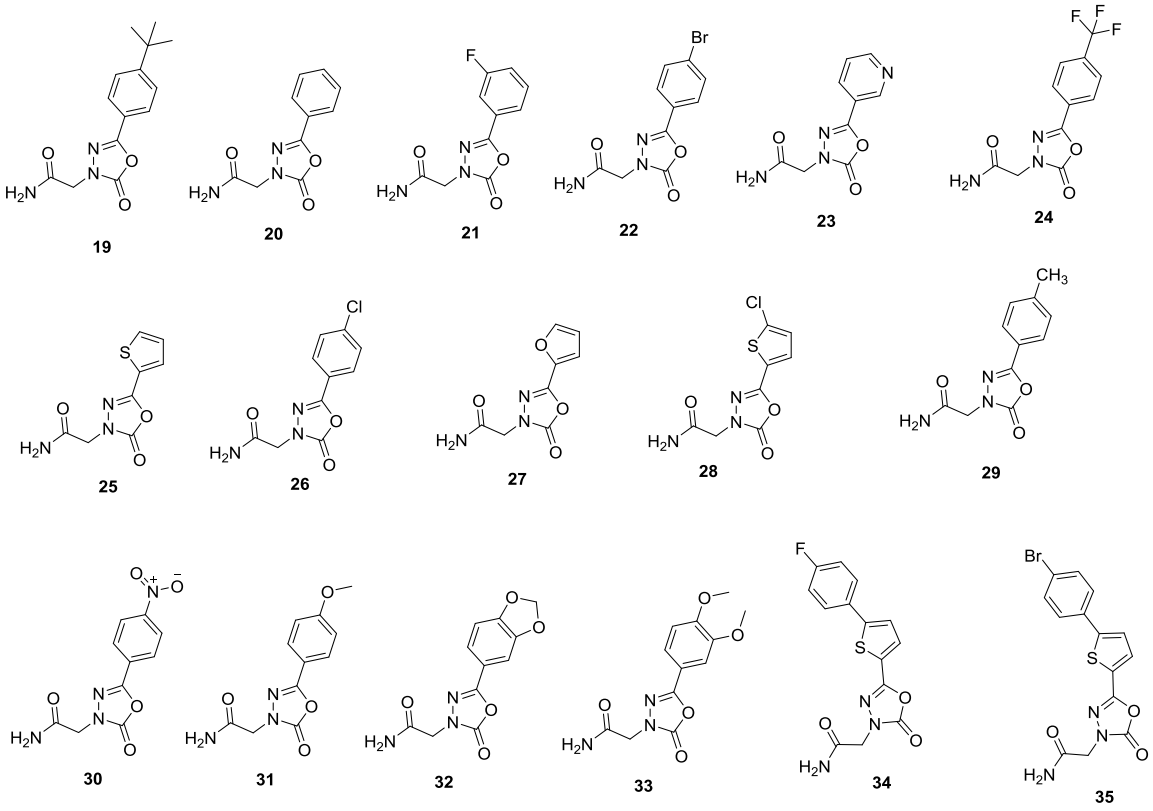
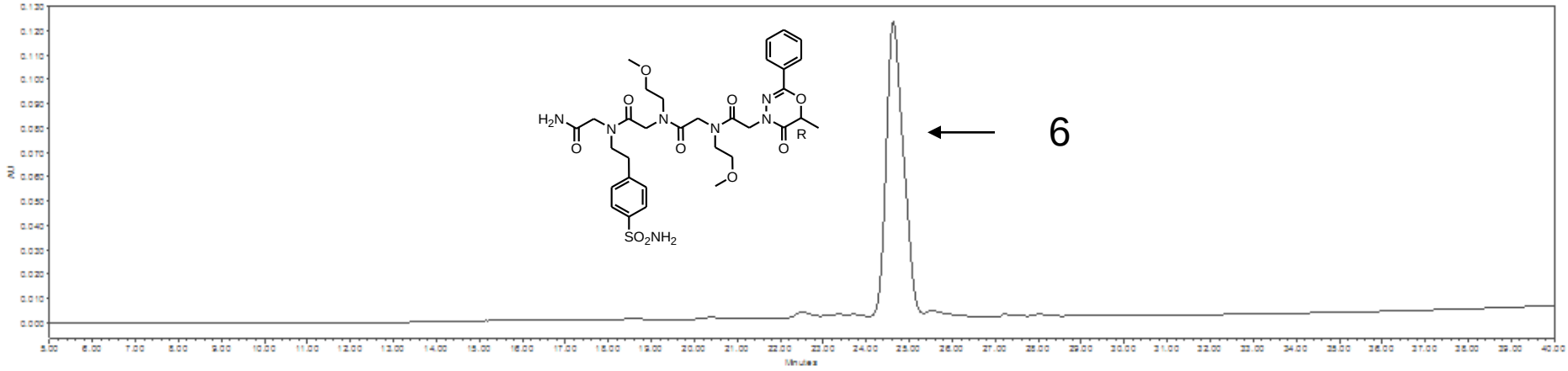


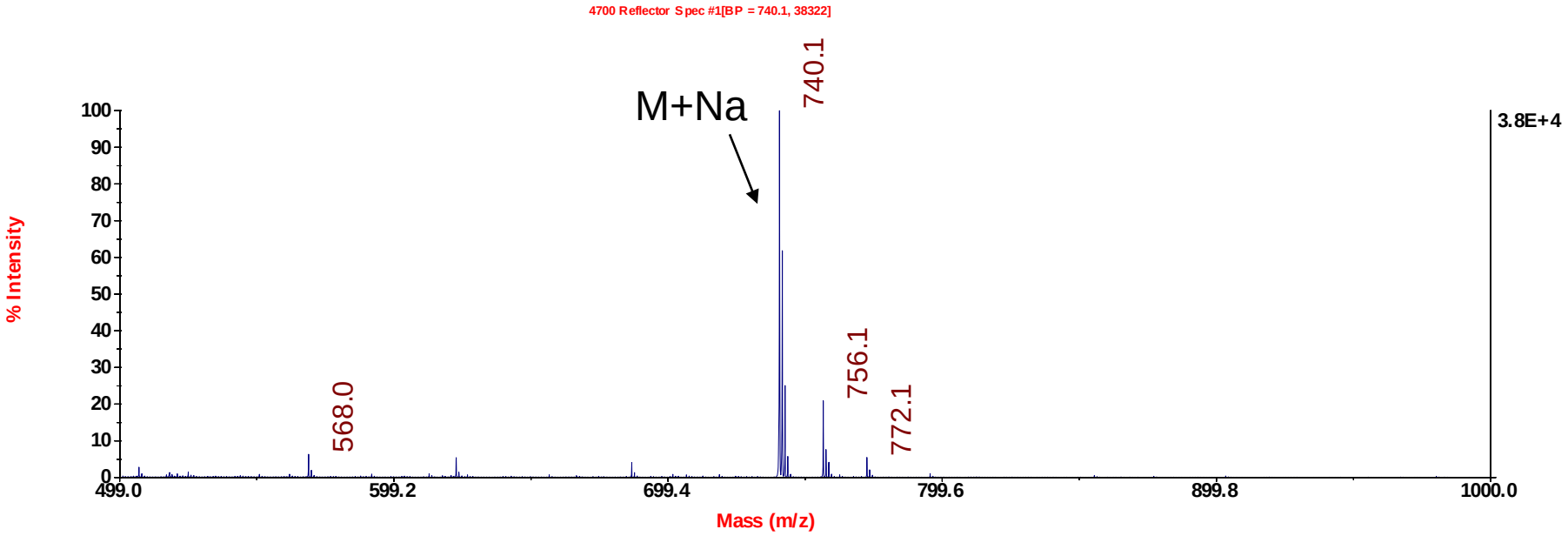
Fig. S6. Chemical structures of 1,3,4-oxadiazol-2-ones **19**-**35**.

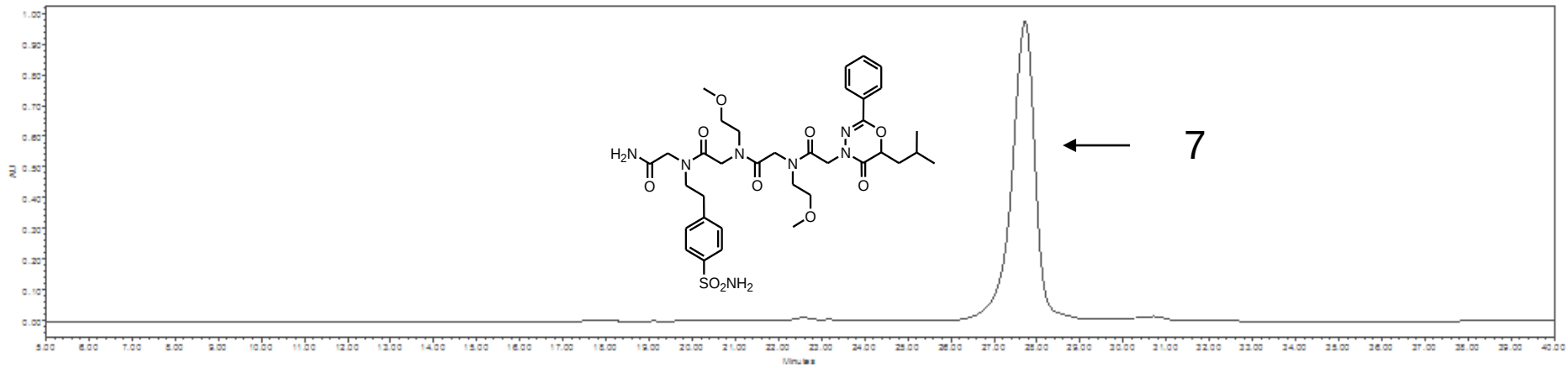
The compounds **19-35** were synthesized on knorr amide MBHA resin (Novabiochem, 0.75 mmol/g). 200 mg beads were soaked in dimethylformamide (DMF) for 1h and then the Fmoc group was deprotected by treating with 4 mL 20% solution of piperidine in DMF for 30 mins. After Fmoc deprotection, the beads were bromoacylated by using 2mL bromoacetic acid (2M) in presence of 2mL diisopropylcarbodiimide (DIC) (3.8M) [overall volume 4mL for 200 mg beads) for 10 mins at 37 °C. The bromoacylated resin beads were then treated with 1M solution (4mL) of the respective acyl hydrazides for 1h at 37 °C. The beads were then washed with DMF and dichloromethane (DCM) and incubated in DCM for 10 mins. DCM were drained and the beads were then treated with 5 equiv. of *p*-nitrophenyl chloroformate (in 2mL anhydrous DCM) and 7 equiv. of diisopropylethylamine (DIEA) (in 2mL DCM) (overall volume 4mL) at room temperature for 3h. The beads were then washed with DCM and DMF and incubated with 4mL of 1M DIEA solution in N-methylpyrrolidione (NMP) at 60 °C for 15h. The beads were then washed with DMF (5 times) followed by DCM (5 times) and then incubated with DCM for 10 mins. The DCM were drained and the compounds were cleaved from the resin by treating with 4mL TFA cocktail [95% TFA, 2.5% trisisopropylsilane (TIPS) and 2.5% water] for 1h. The TFA solution was collected and then evaporated by blowing argon. The compounds were then precipitated by treating with cold ether and centrifuged. The ether were decanted and the precipitate was subjected to preparative HPLC to obtain pure **19-35** in >95% yield. However, our attempt to synthesize compound **36** failed under these conditions. The only product observed from this reaction was compound **37**.

ABPP Gel-based activity assay: The purified serine hydrolase (2 μM; PAFAH1b2, PAFAH1b3, FAM108B, PME-1, or RBBP9) or cell lysate (1mg/mL) doped with 100-200 nM purified protein was incubated in assay buffer [50 mM Tris-HCl (pH 8) and 150 mM NaCl] containing the potential inhibitor at varying concentrations. The reaction was incubated at r.t. for 30 mins before the addition of a fluorophosphonate-rhodamine (FP-Rh) probe. After 30 mins (10 mins for cell lysate), the reaction was quenched with a 6X SDS dye, heated at 95°C for 10 minutes, and analyzed by SDS-PAGE. The fluorescence was visualized in-gel using a Typhoon imager.

Figure S7: HPLC and MALDI TOF mass spectra of compounds **6-13.**



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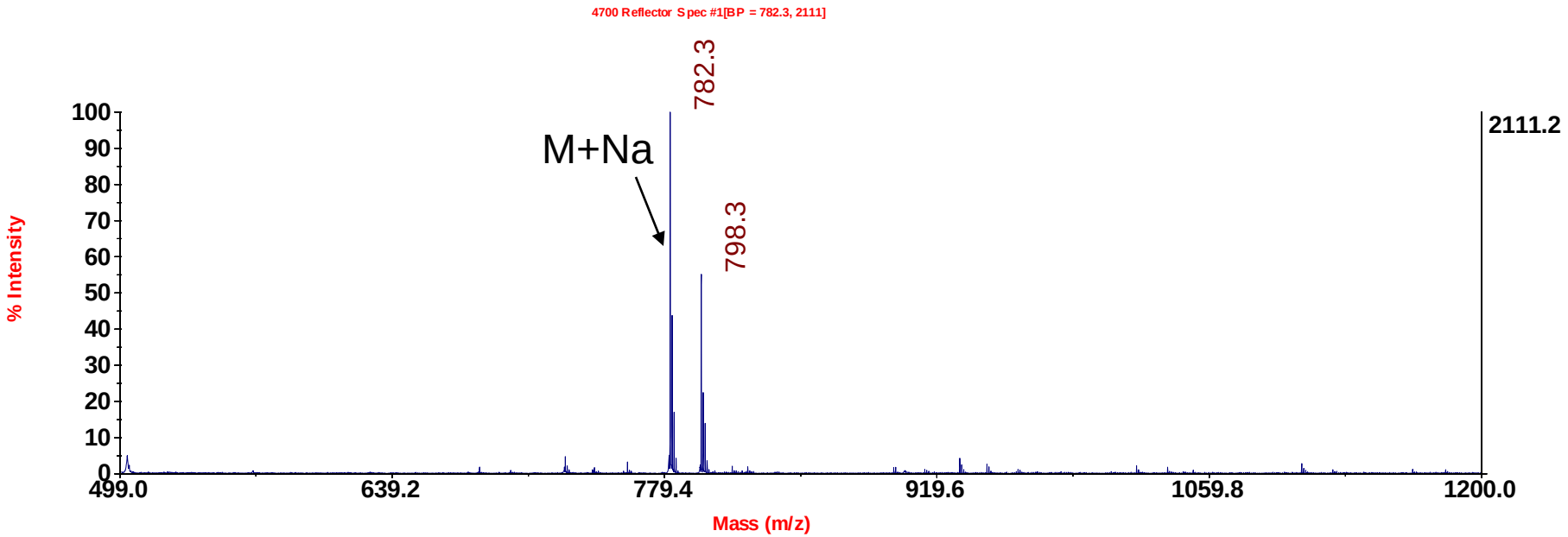
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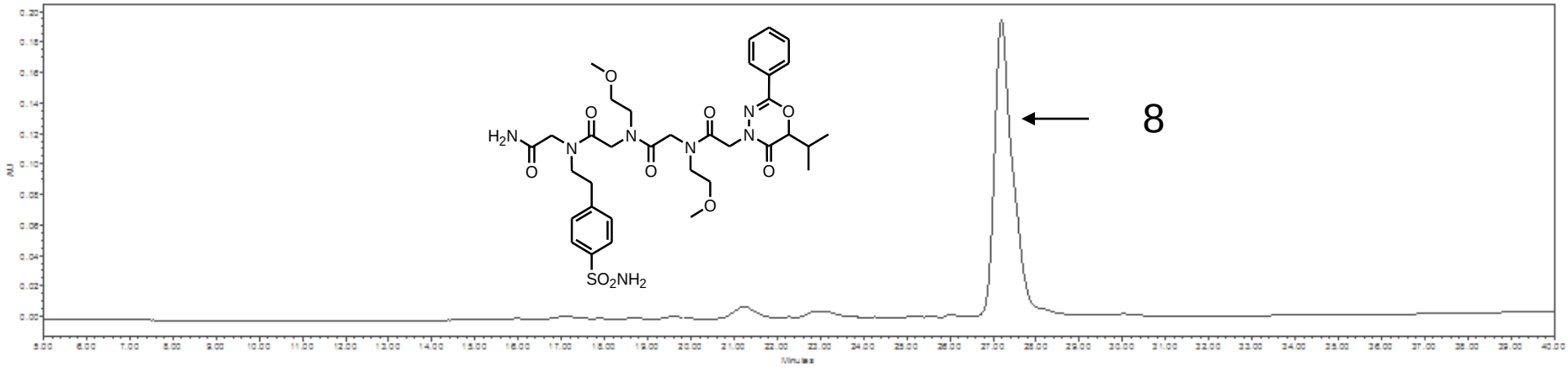
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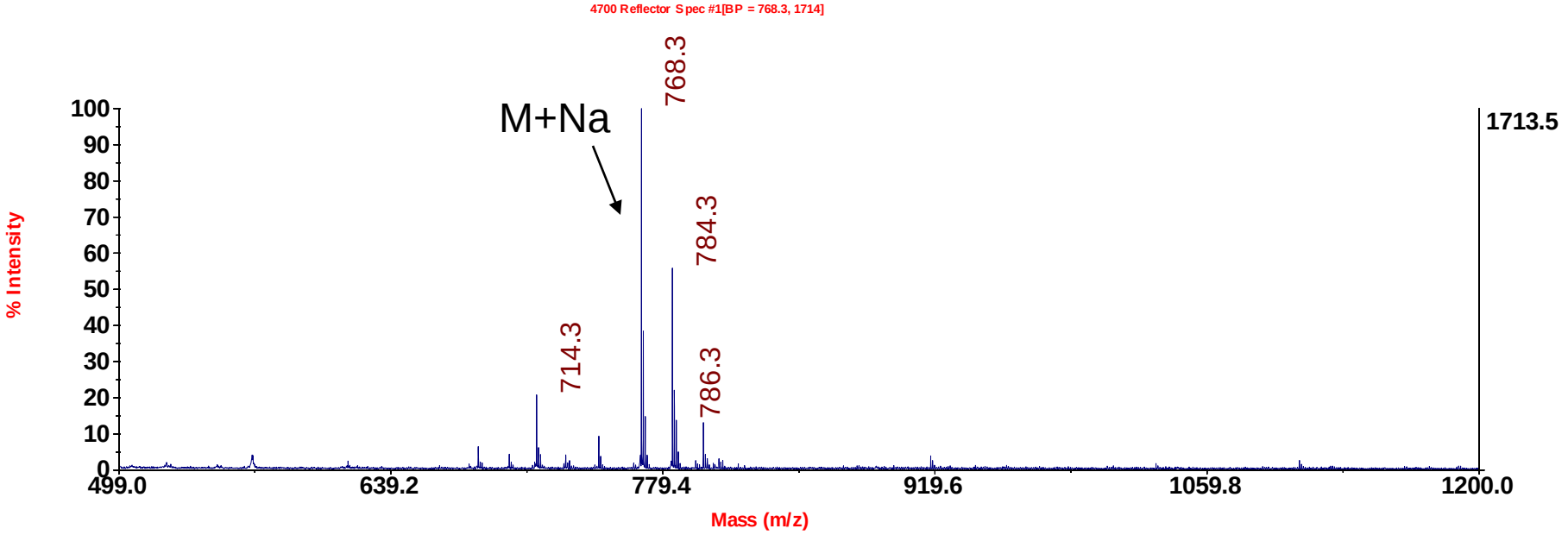
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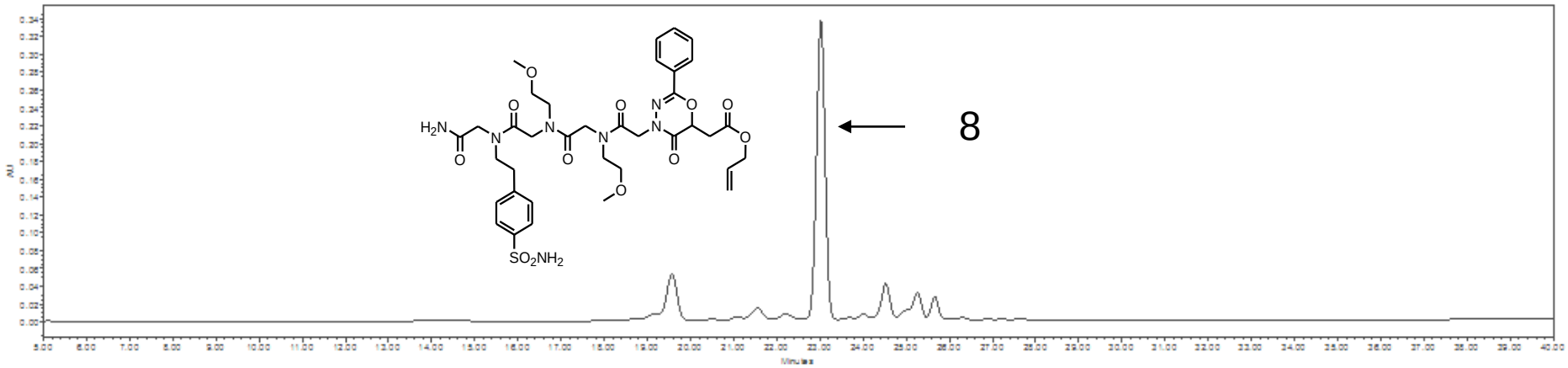
779.4
919.6
1059.8
1200.0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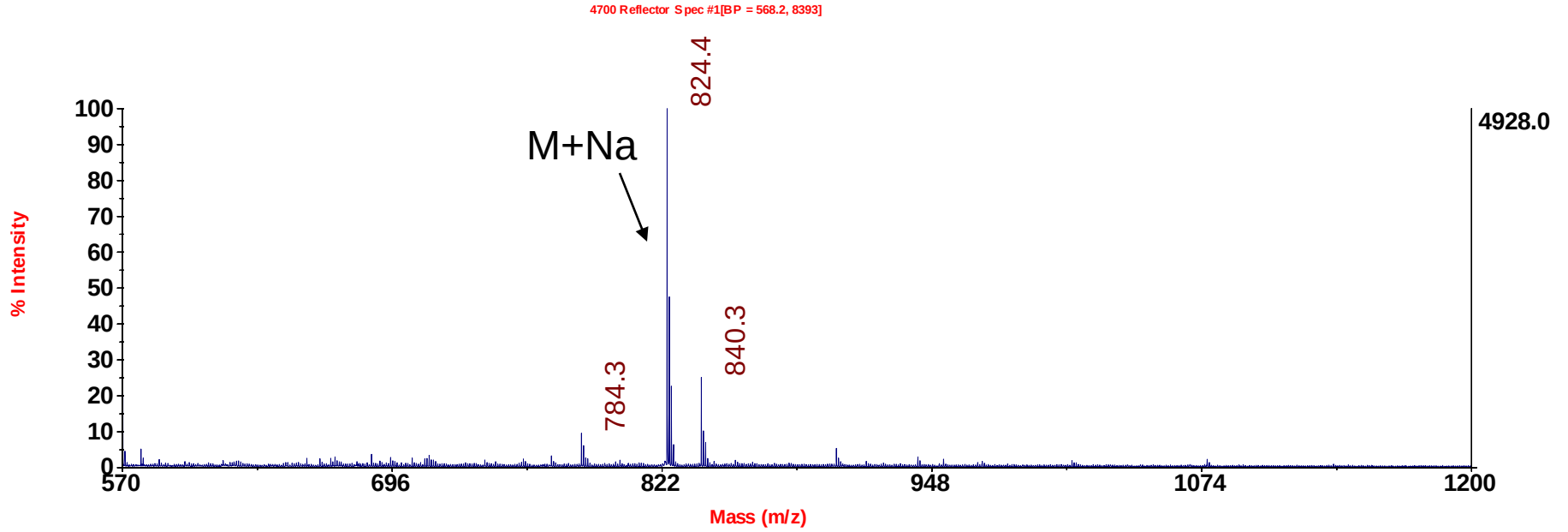
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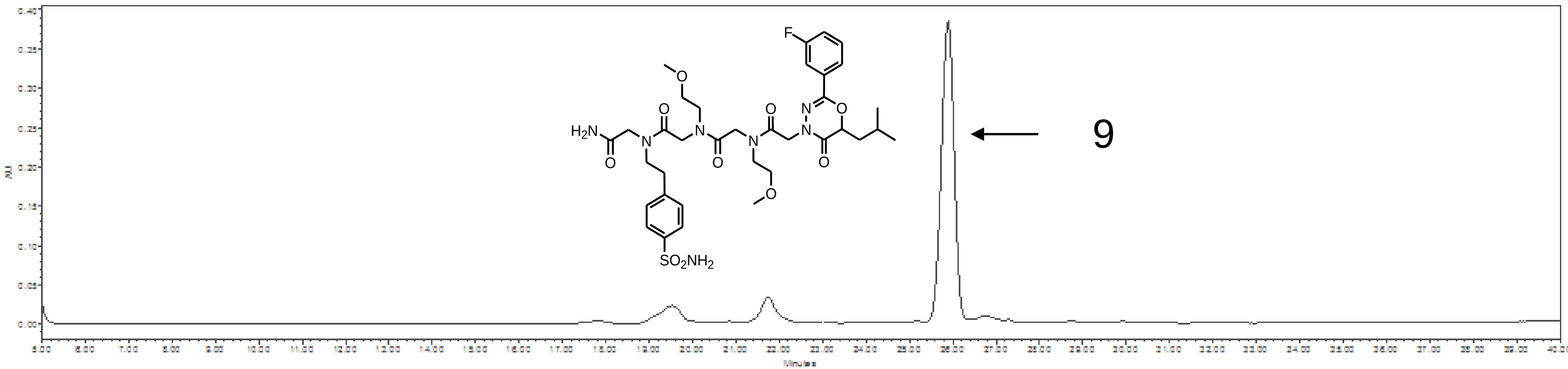
948
1074
1200
Mass (m/z)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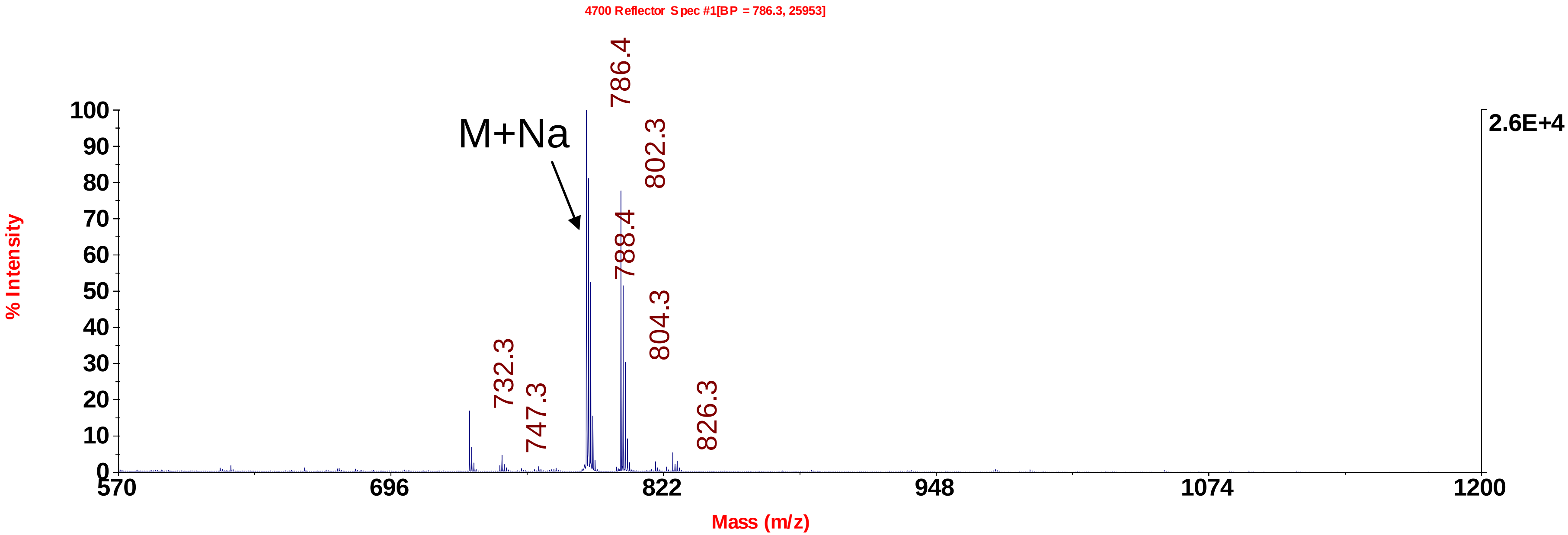
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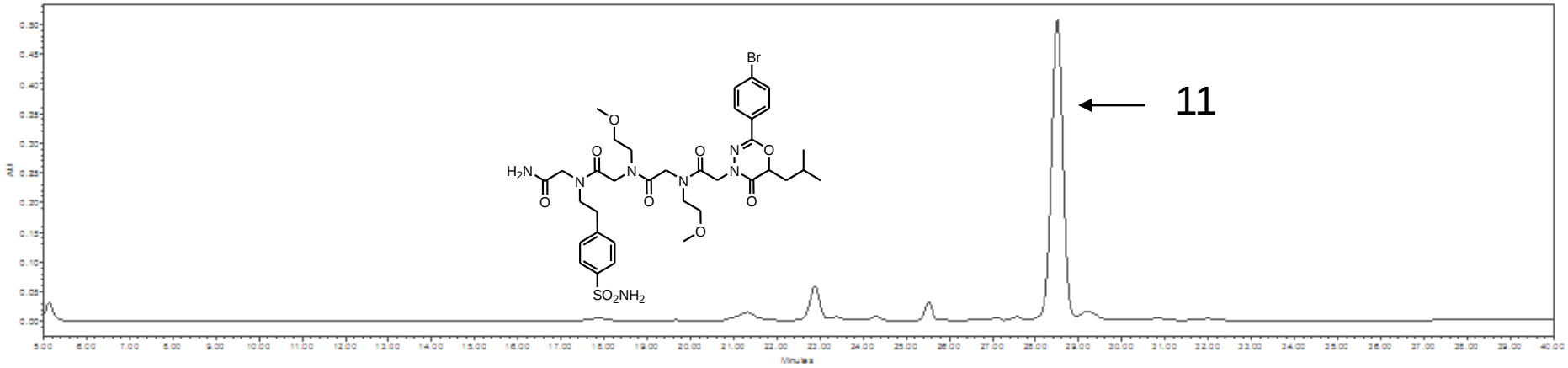

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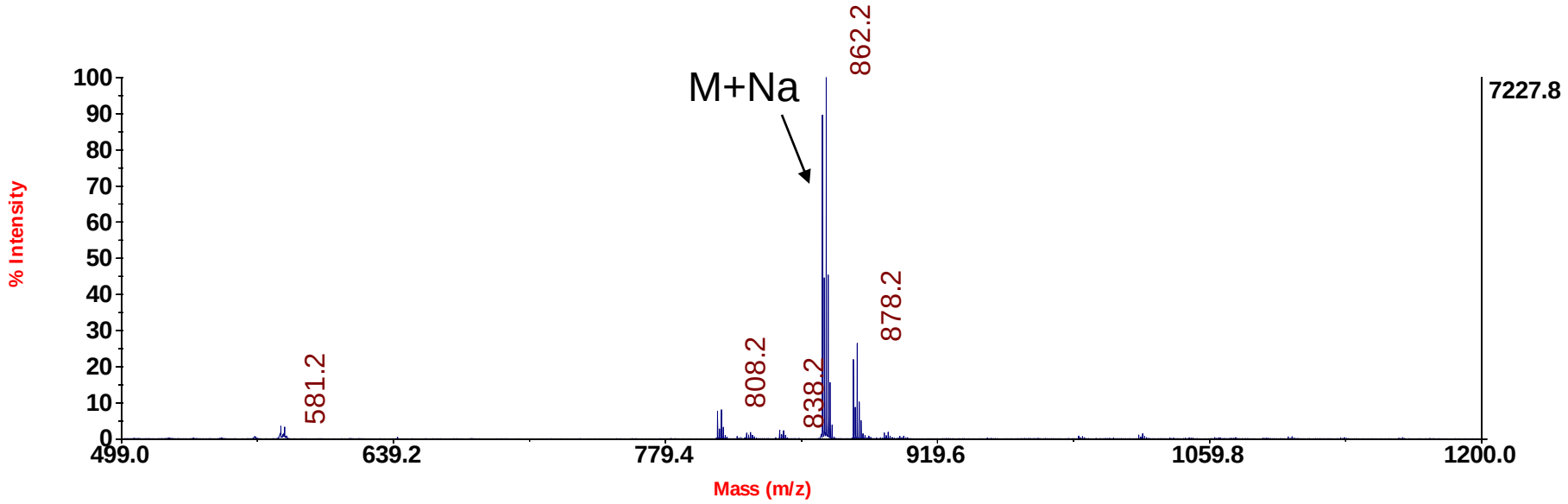

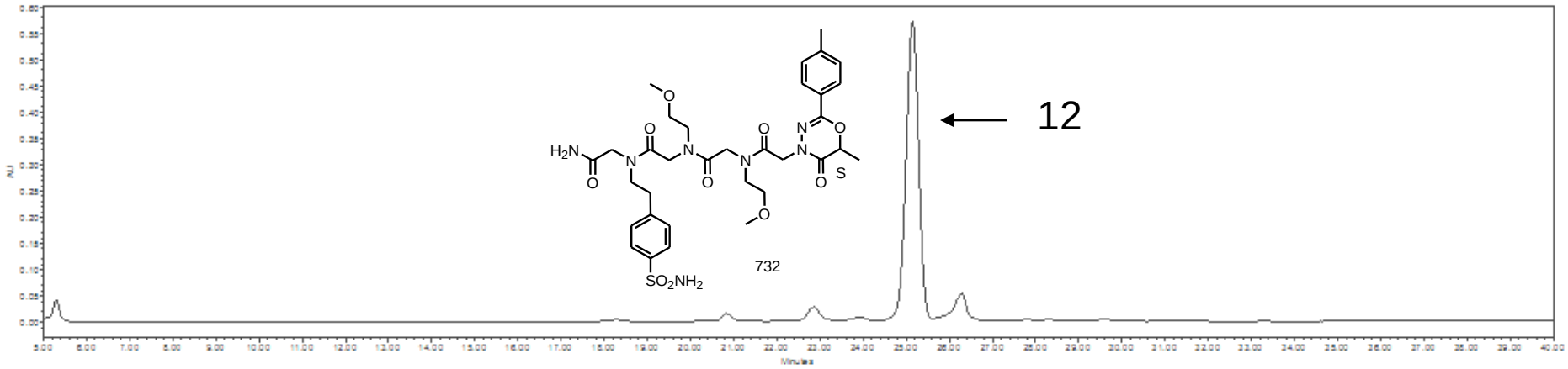
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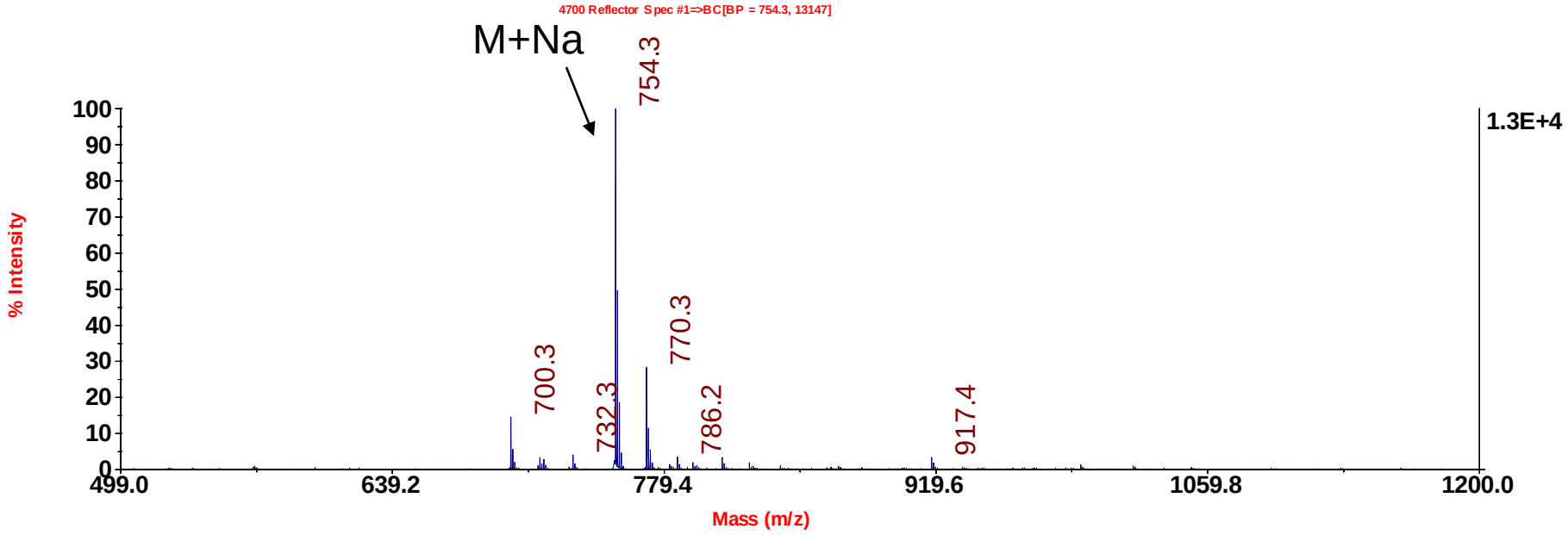
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1.3E+4
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Mass (m/z)
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40
30
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10
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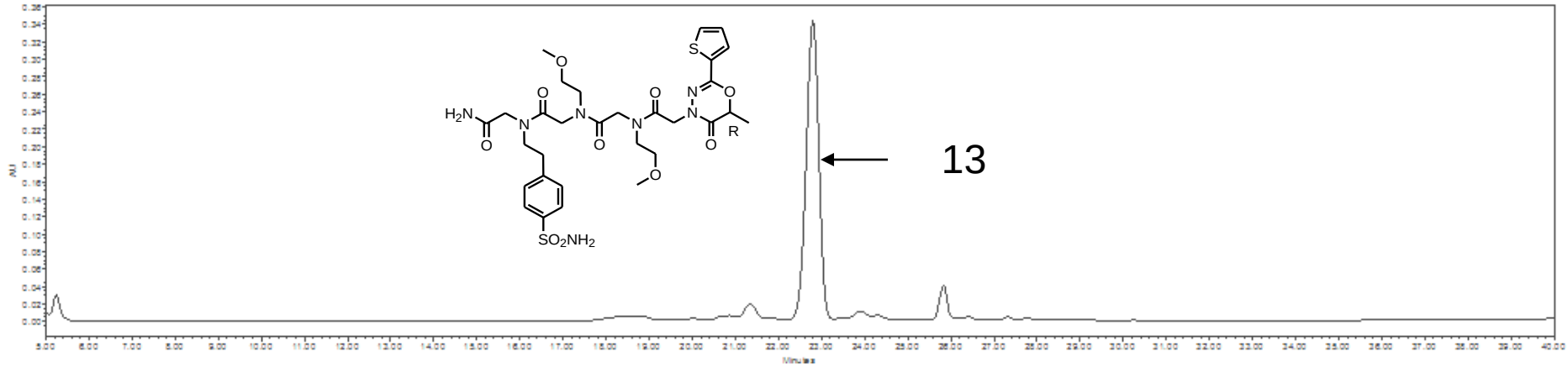
779.4
919.6
1059.8
1200.0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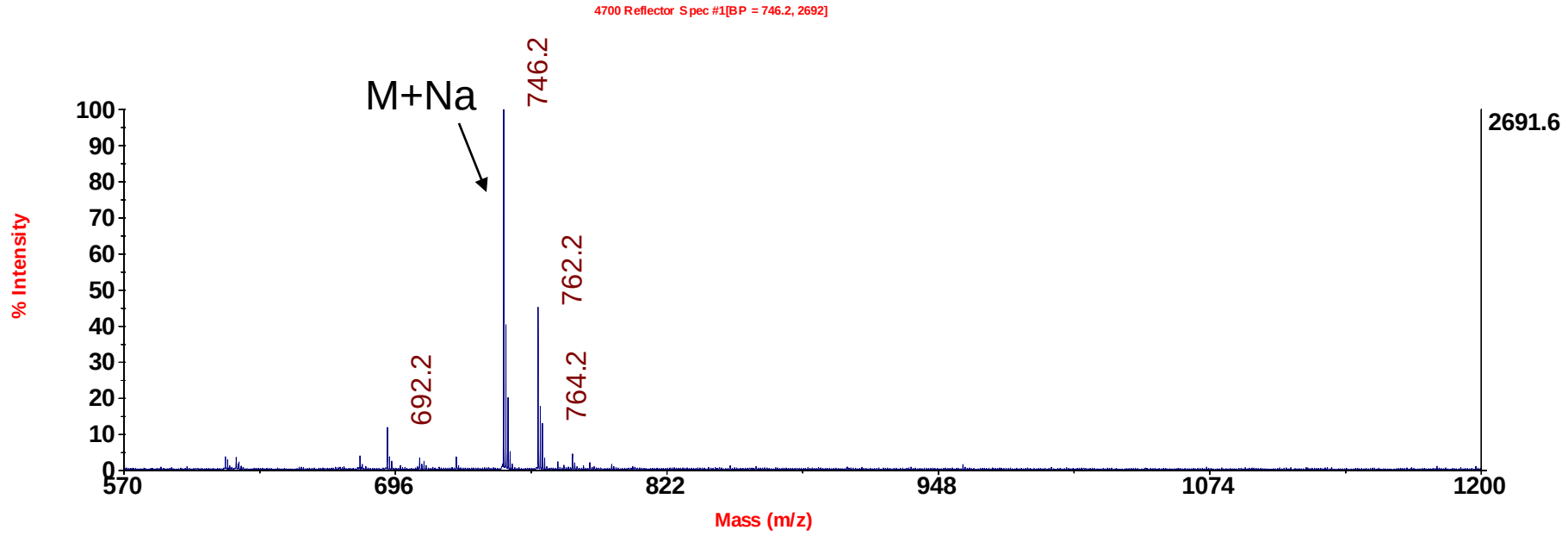
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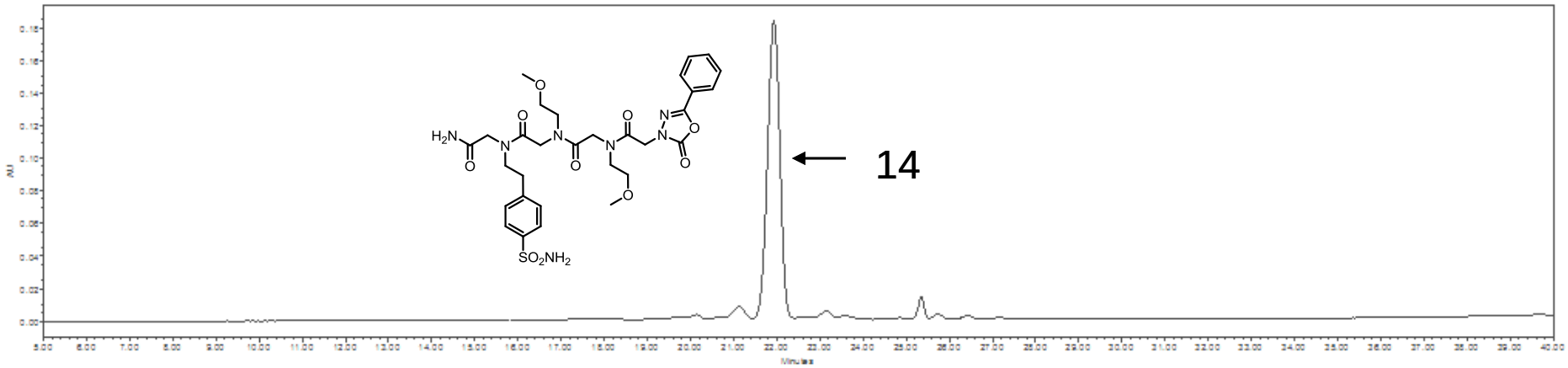
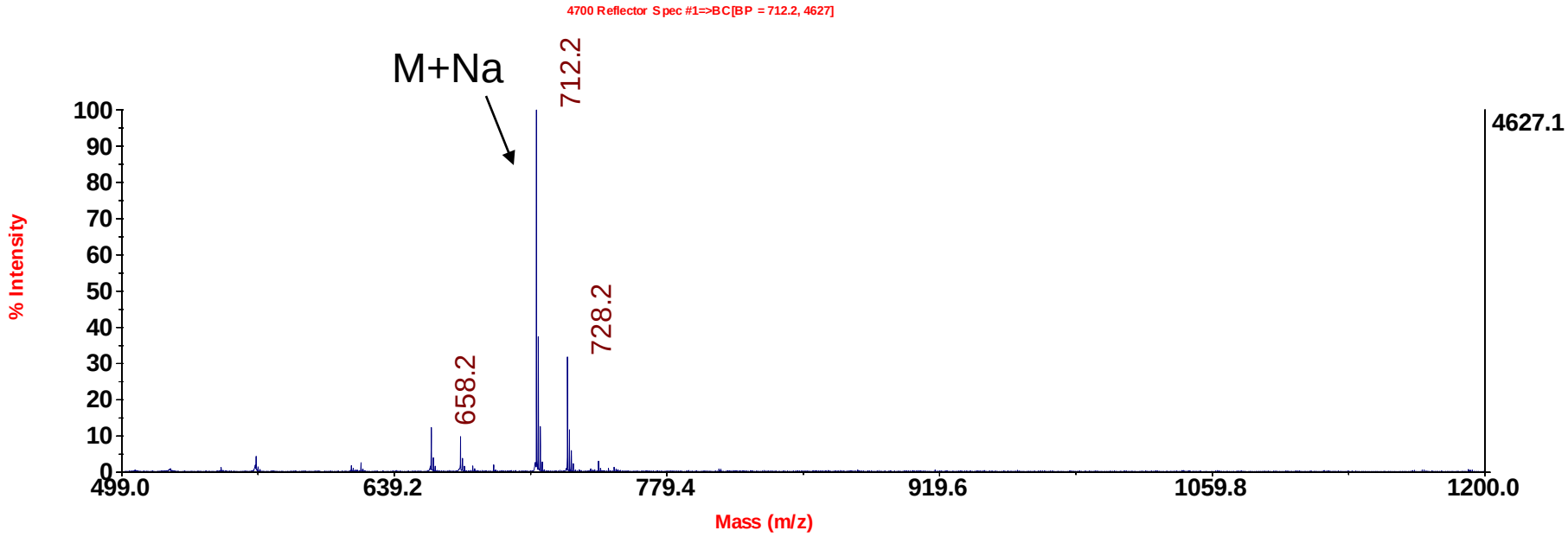
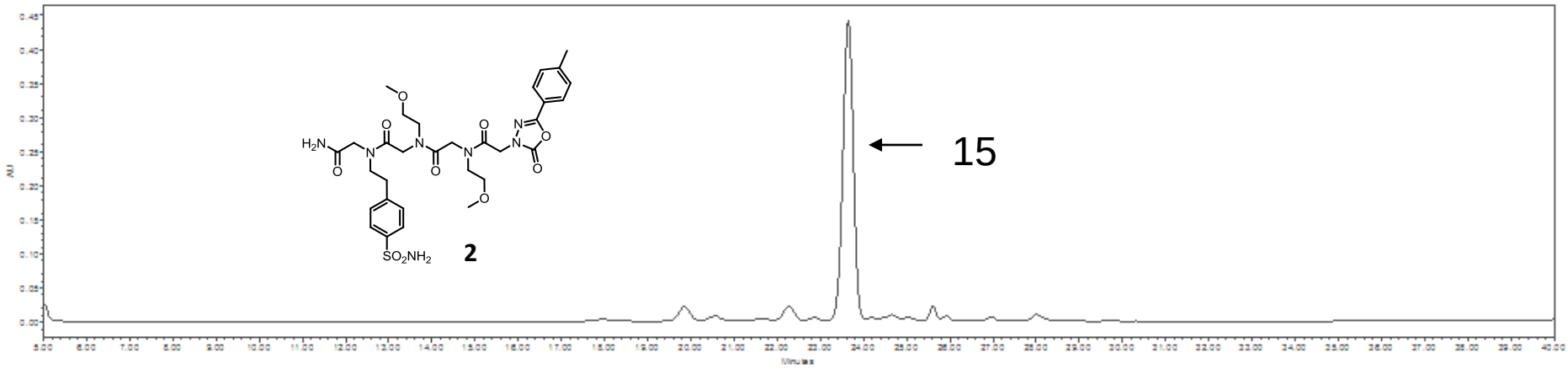
822
948
1074
1200

Figure S8: HPLC and MALDI TOF mass spectrum of compounds **14**-**18**



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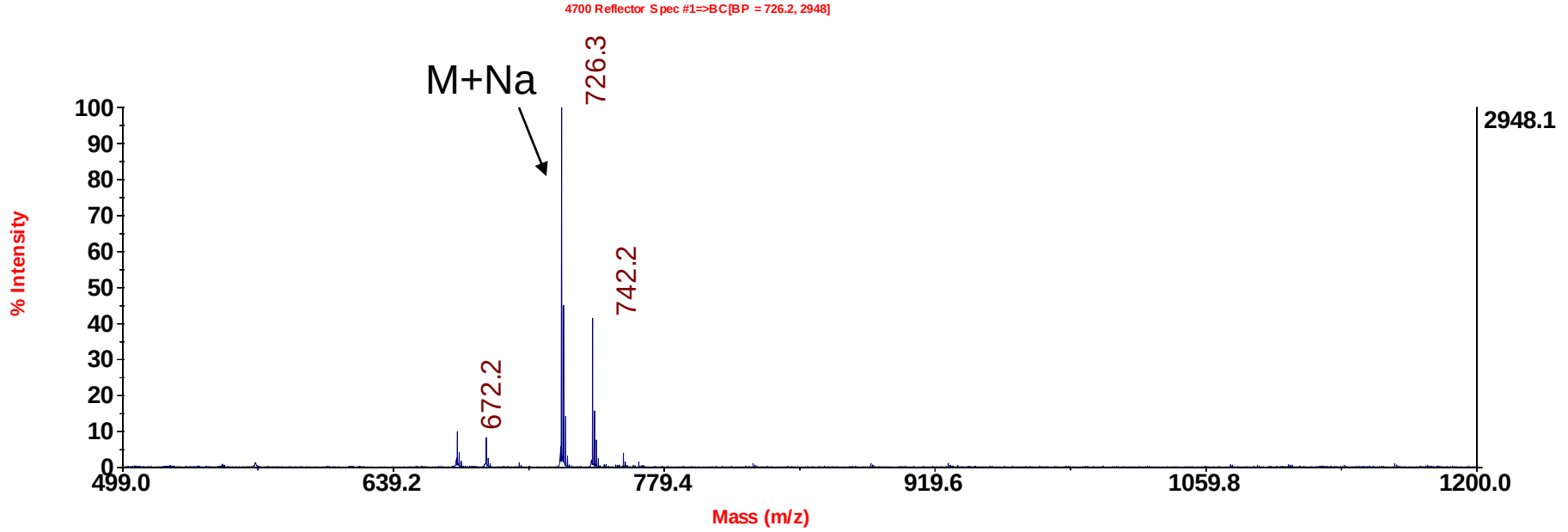
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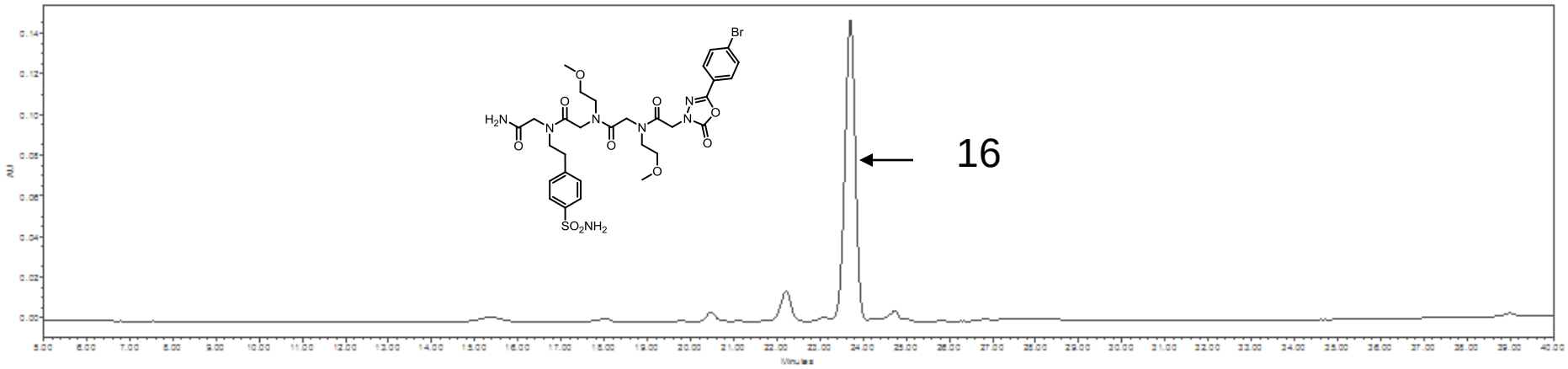
779.4
919.6
1059.8
1200.0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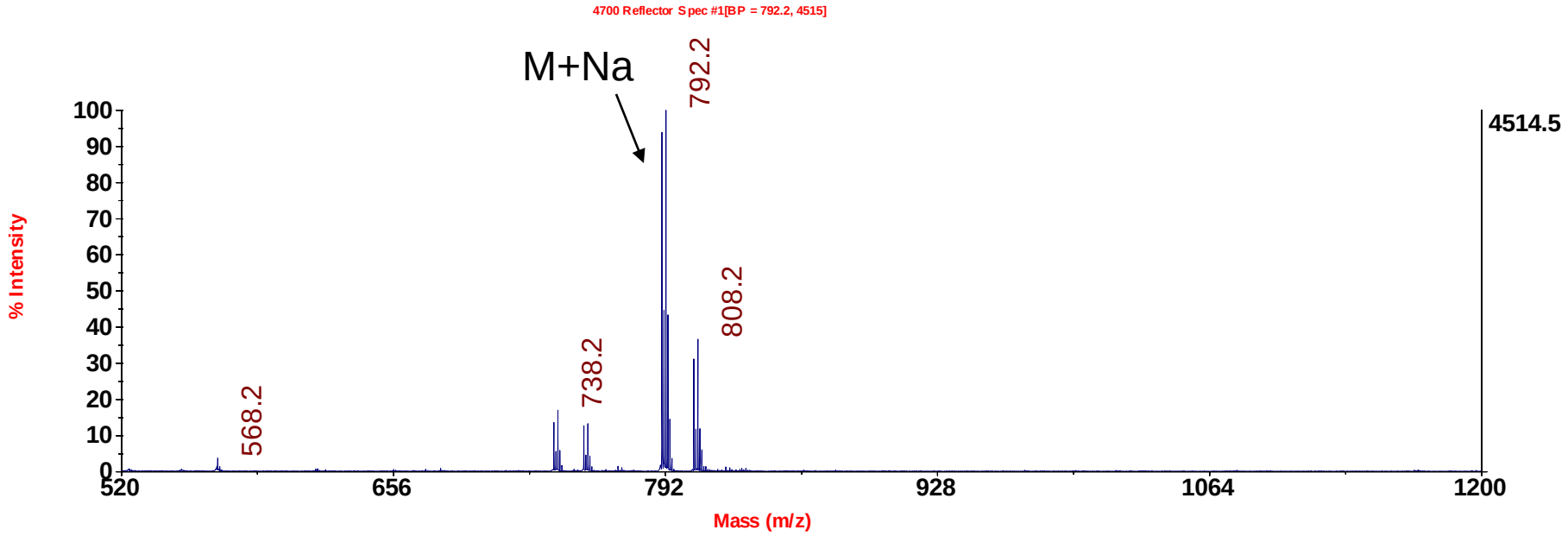
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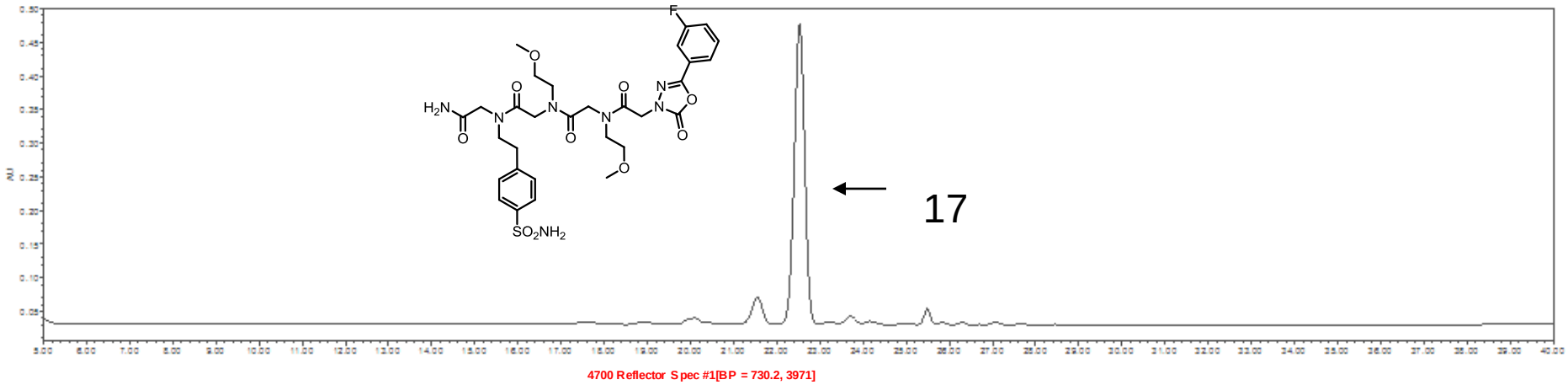
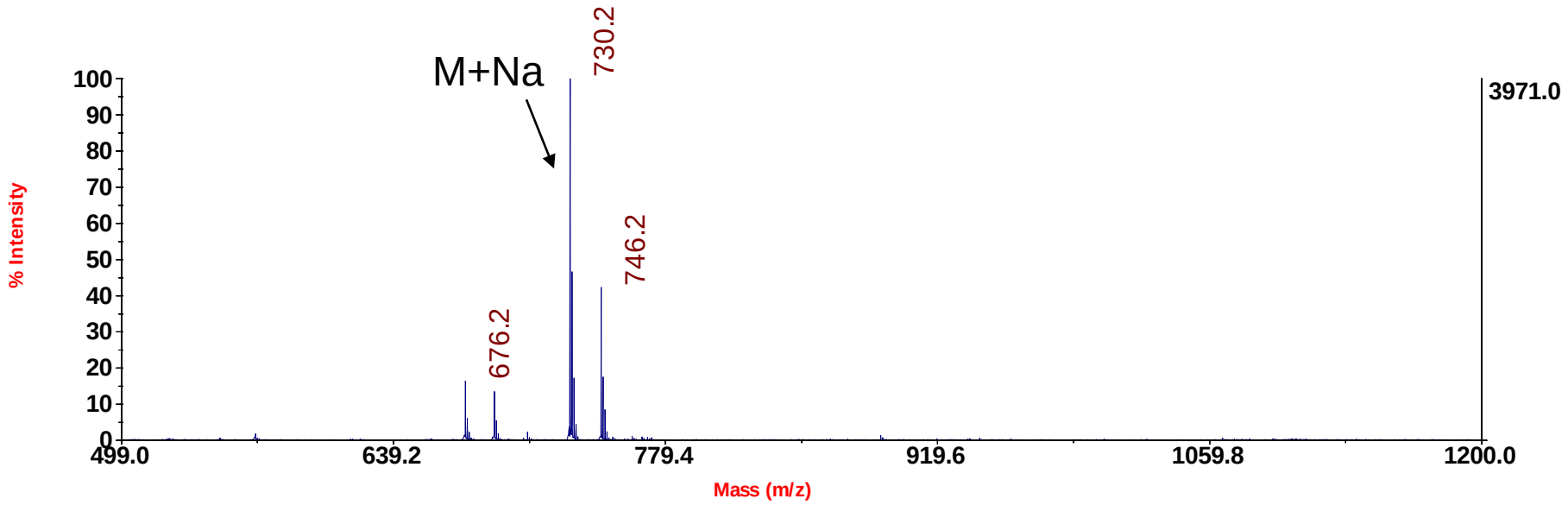
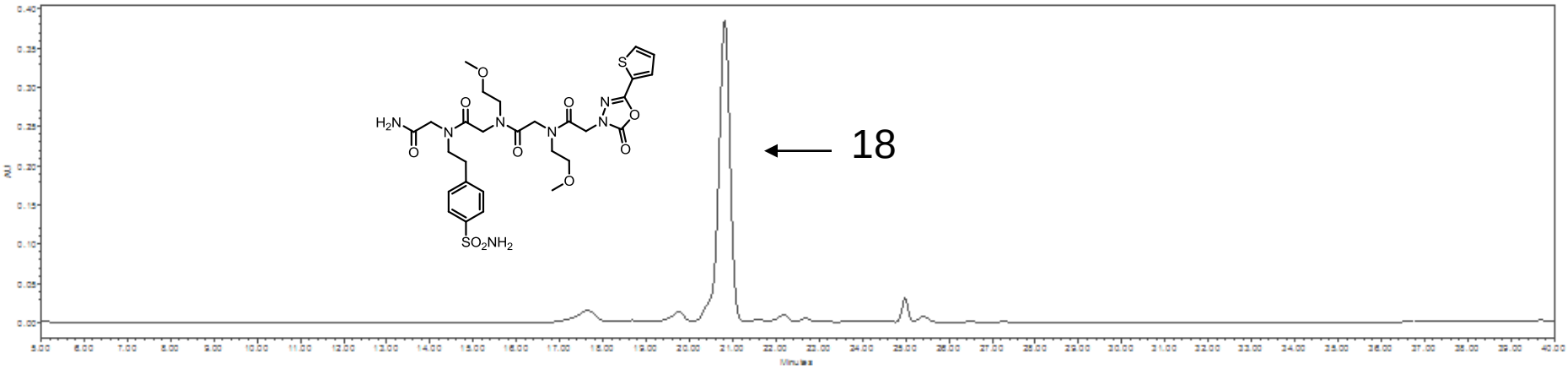
60
50
40
30
20
10
0
520
656
792
928
1064
1200



4700 Reflector Spec #1[BP = 730.2, 3971]




18

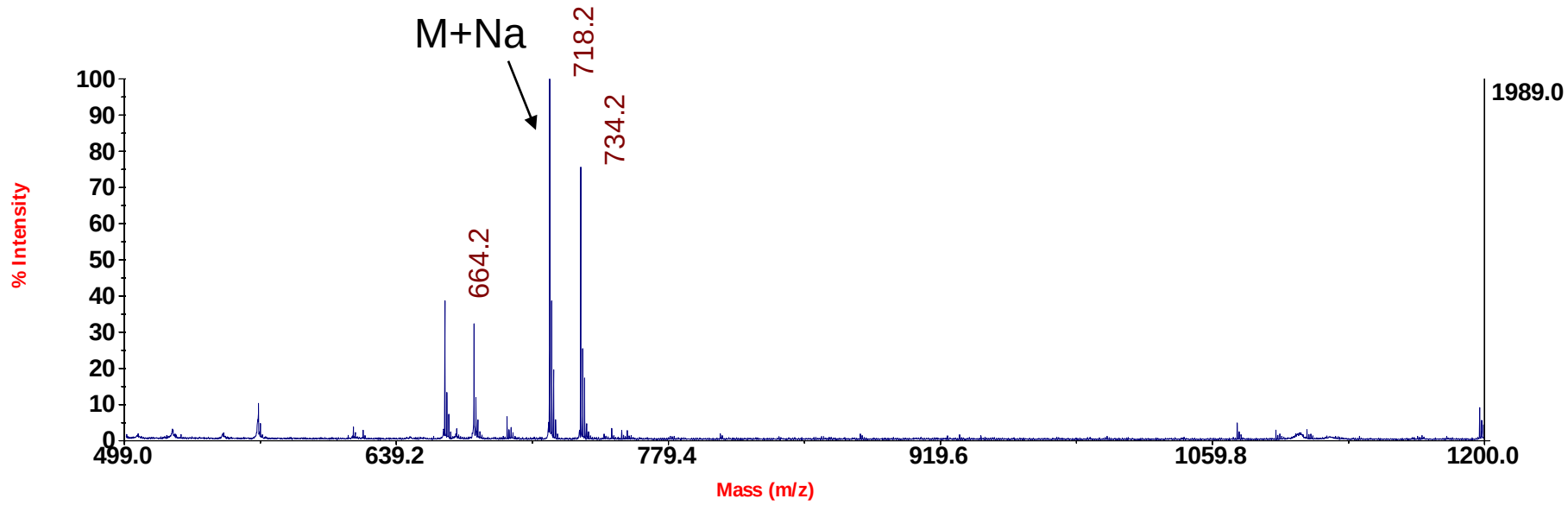
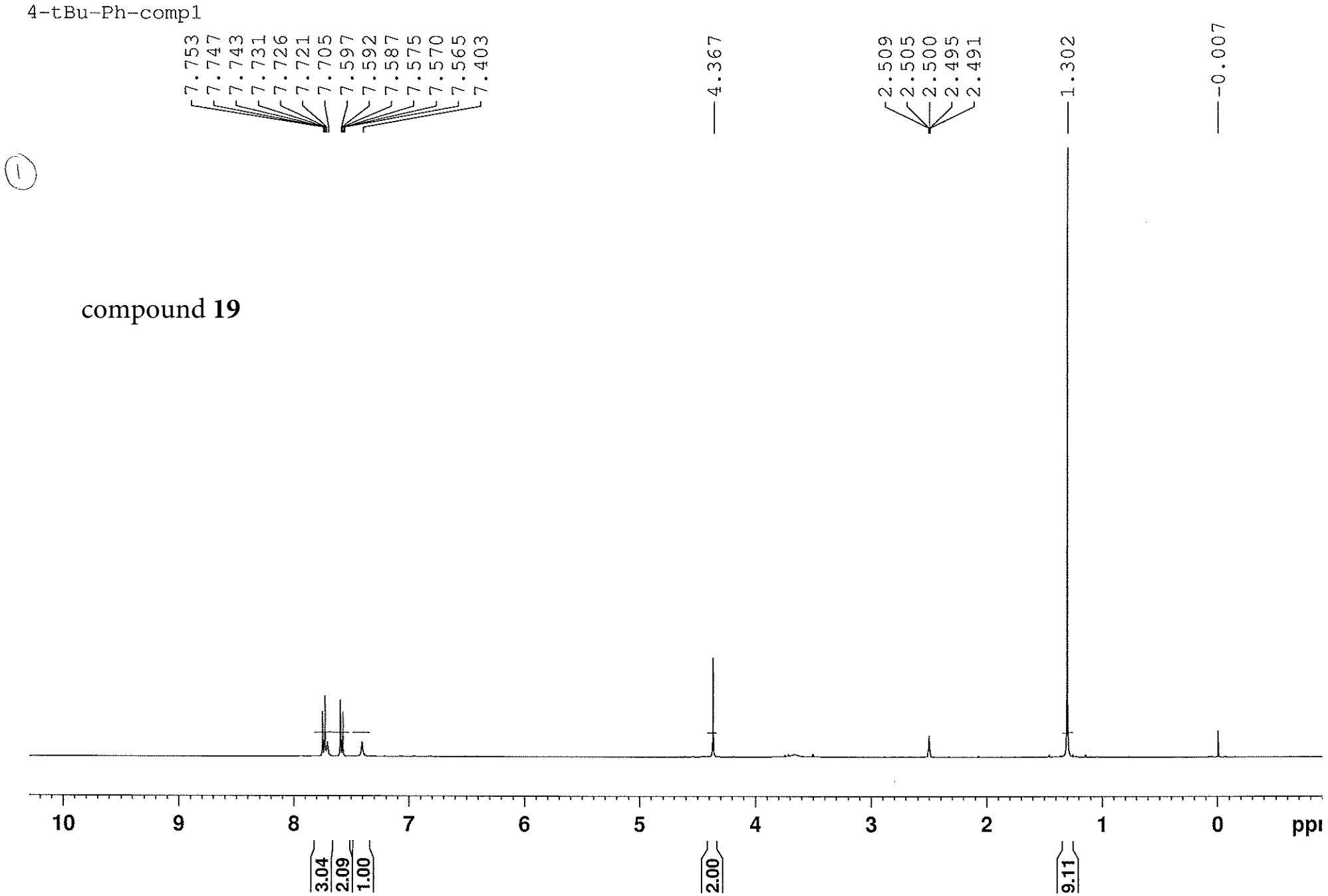
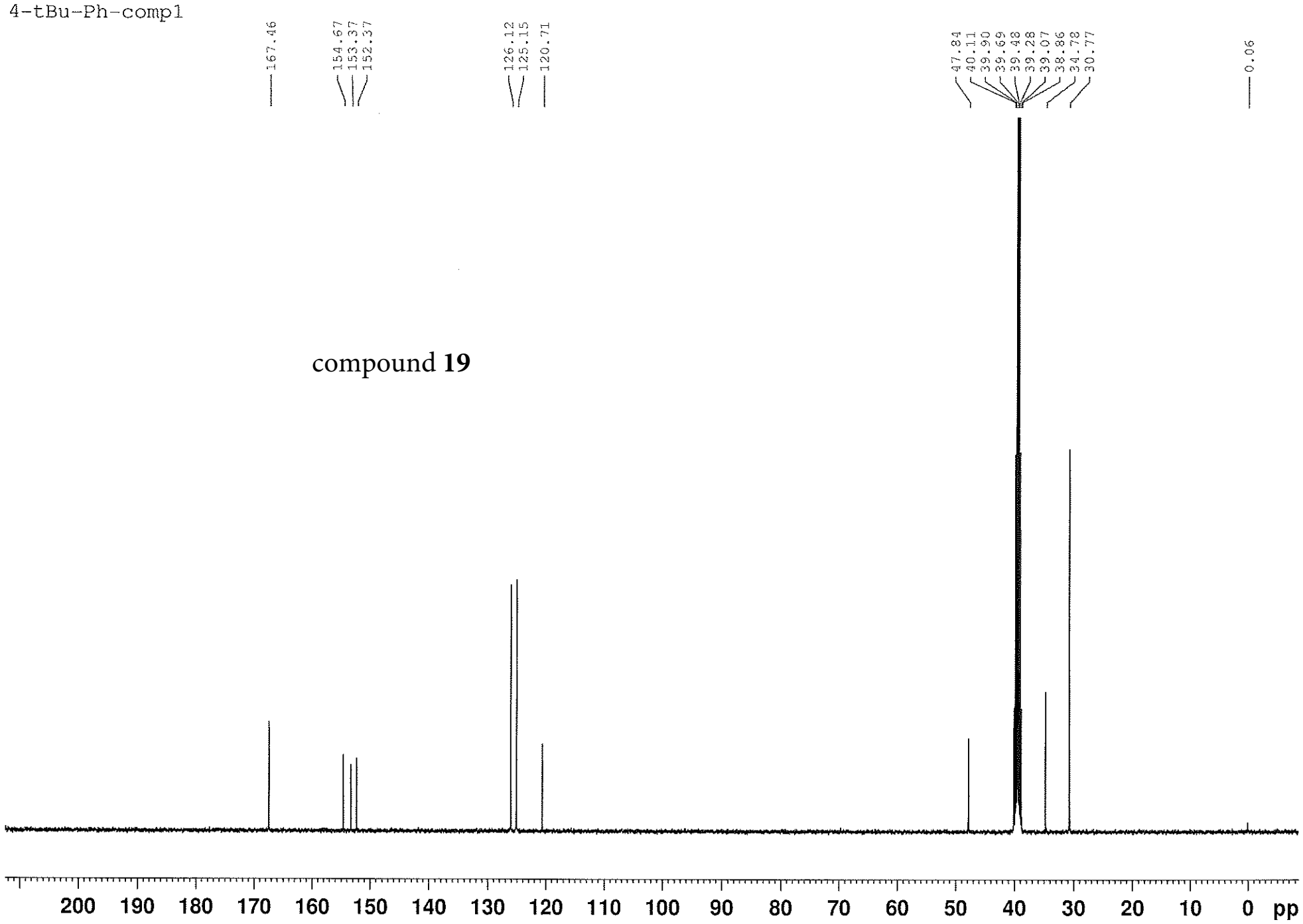

4700 Reflector Spec #1[BP = 718.2, 1989]
M+Na
718.2
734.2
664.2
1989.0
% Intensity
Mass (m/z)
100
90
80
70
60
50
40
30
20
10
0
499.0
639.2
779.4
919.6
1059.8
1200.0

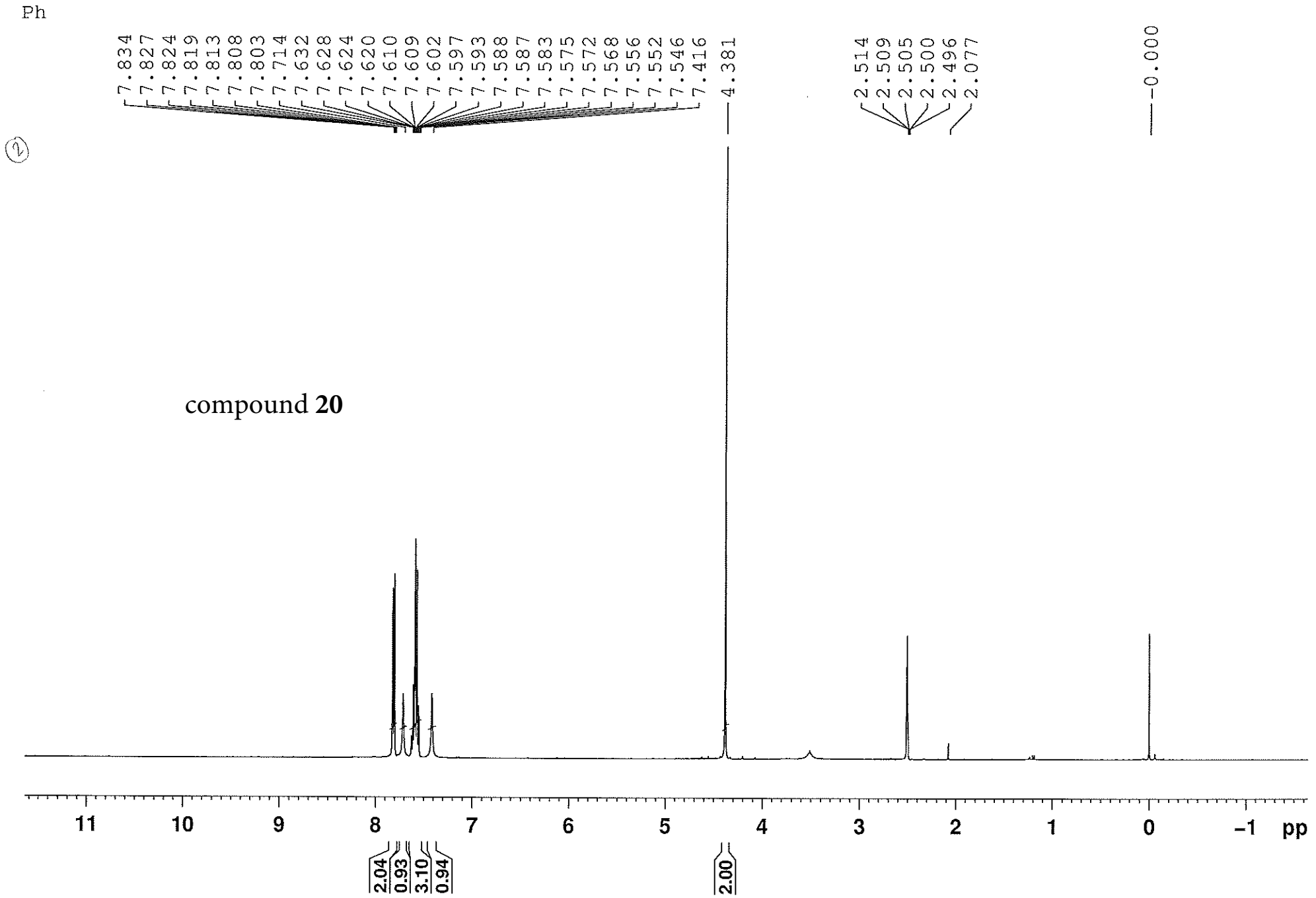
Figure S9: ^{1}H and ^{13}C NMR spectra of compounds **19**-**35** and **37**.

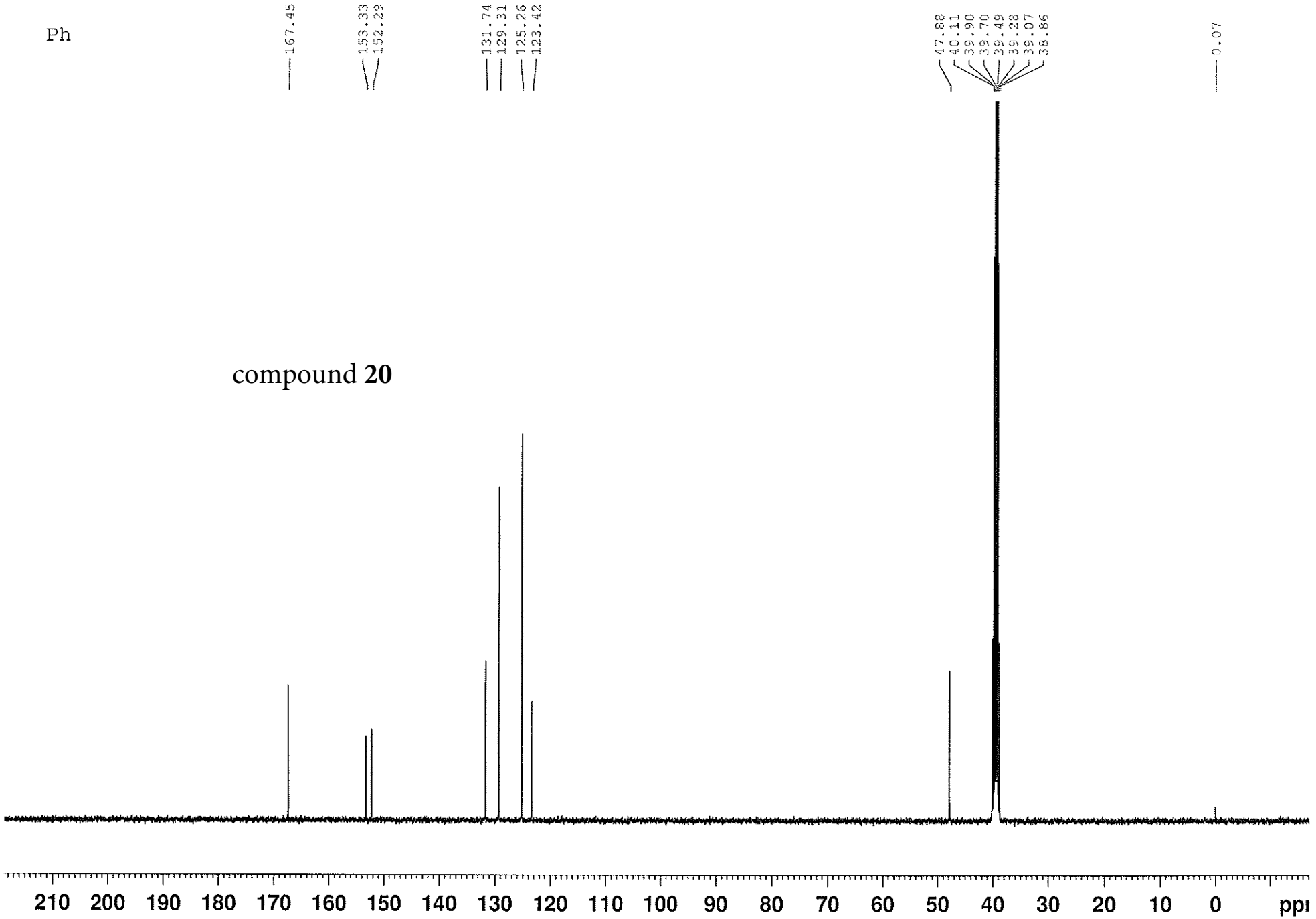


compound **19**

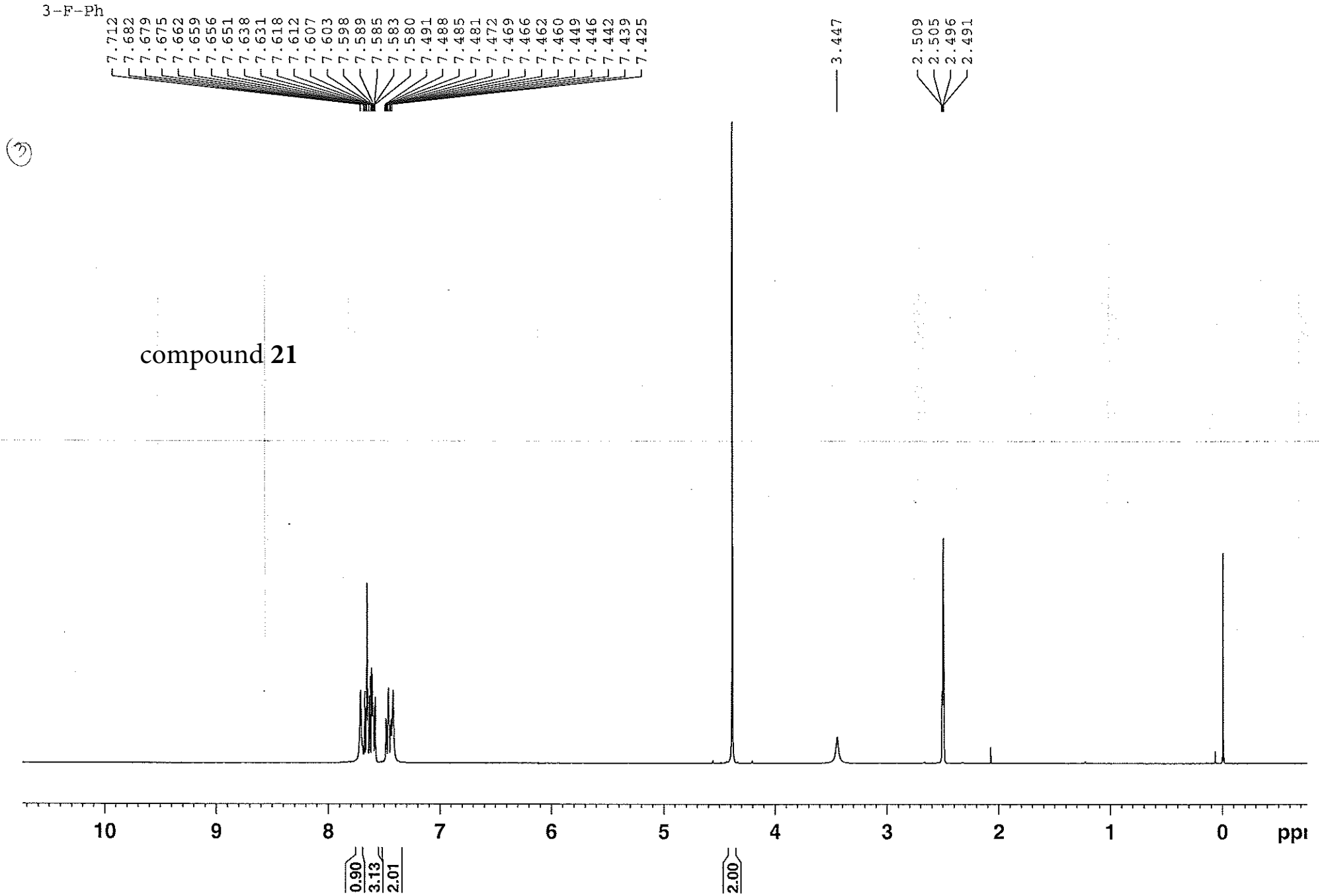

4-tBu-Ph-comp1
167.46
154.67
153.37
152.37
126.12
125.15
120.71
47.84
40.11
39.90
39.69
39.48
39.28
39.07
38.86
34.78
30.77
0.06
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 pp

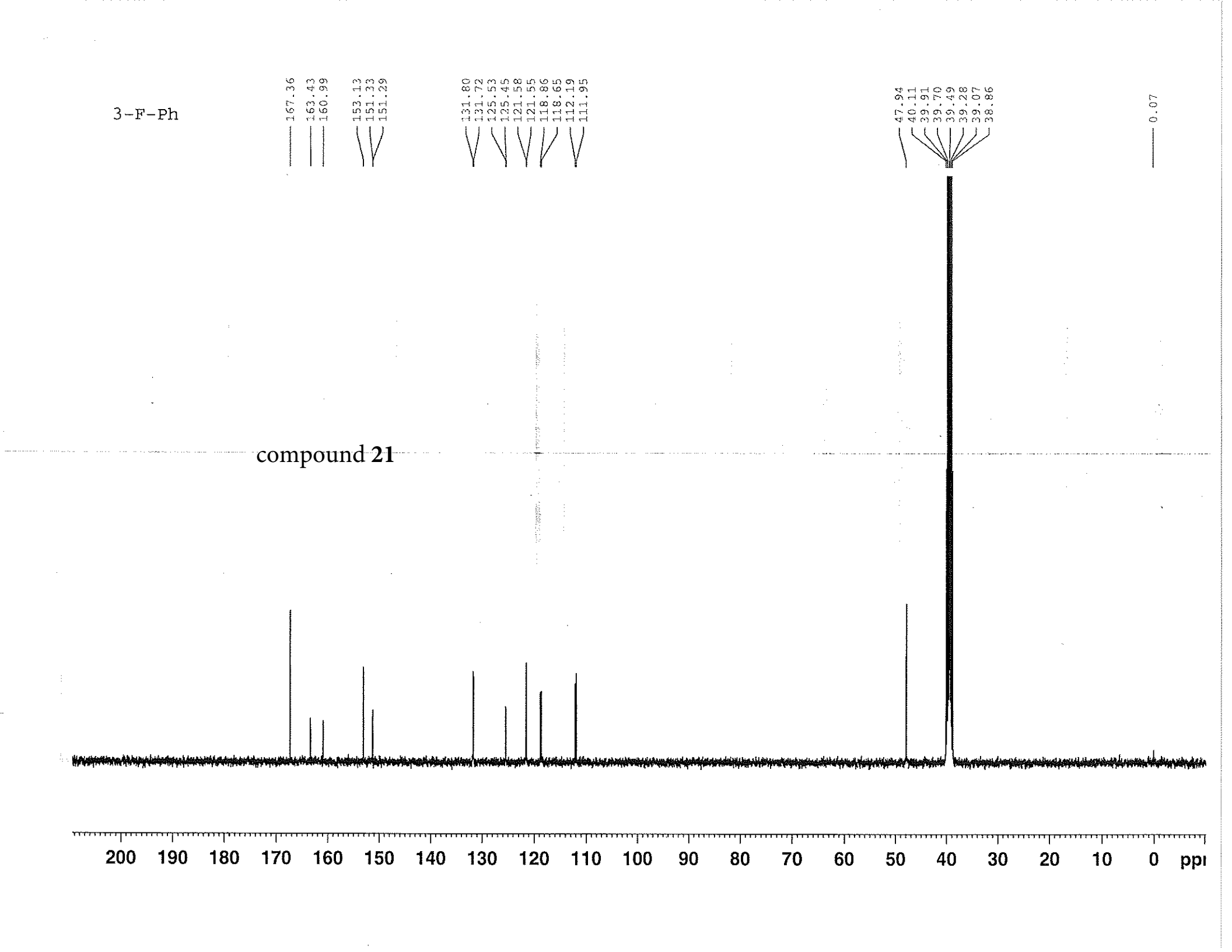
compound **19**


Ph
7.834
7.827
7.824
7.819
7.813
7.808
7.803
7.714
7.632
7.628
7.624
7.620
7.610
7.609
7.602
7.597
7.593
7.588
7.587
7.583
7.575
7.572
7.568
7.556
7.552
7.546
7.416
4.381
2.514
2.509
2.505
2.500
2.496
2.077
0.000
compound 20
11
10
9
8
7
6
5
4
3
2
1
0
−1
pp
2.04
0.93
3.10
0.94
2.00

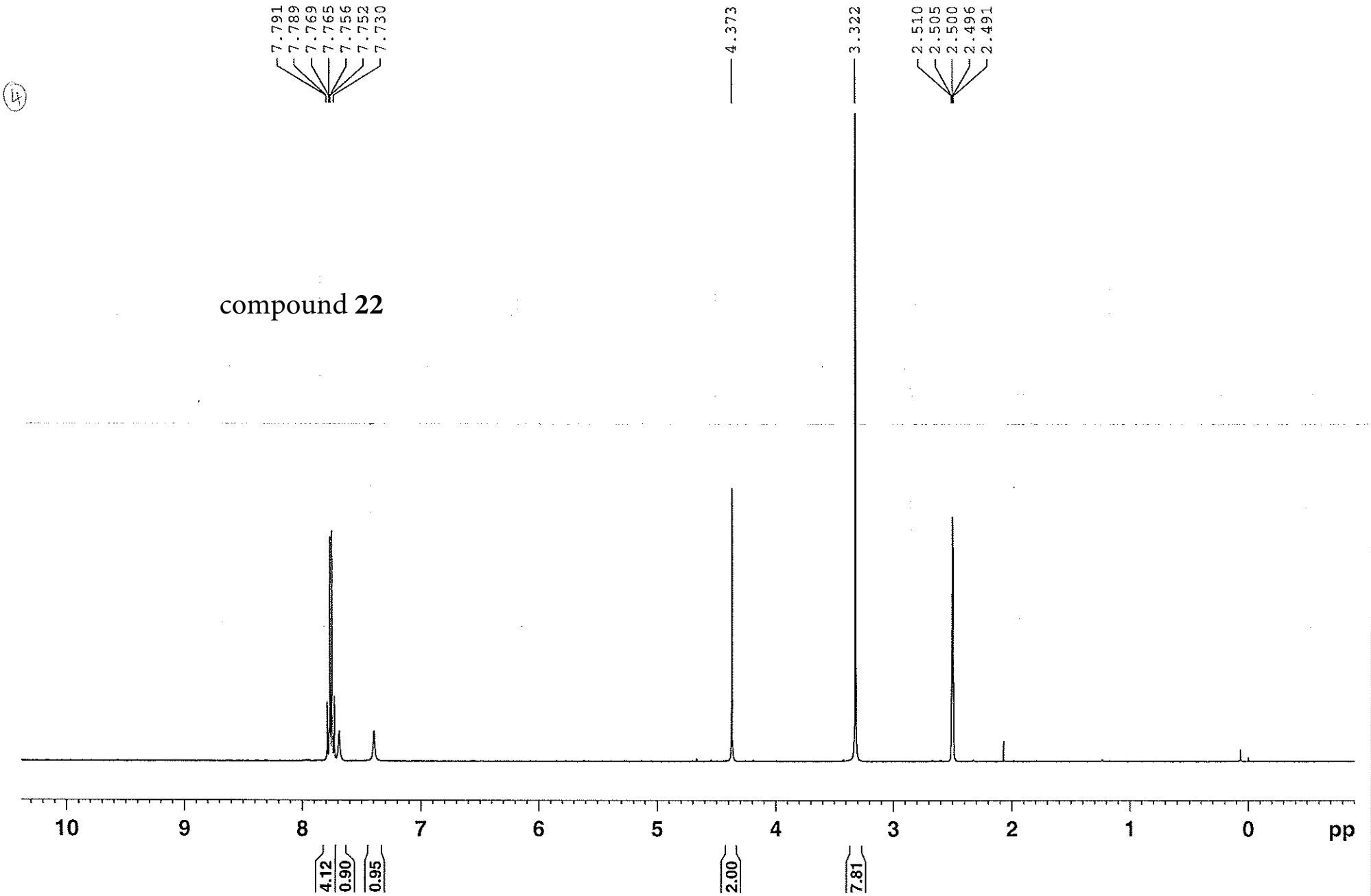

Ph
167.45
153.33
152.29
131.74
129.31
125.26
123.42
47.88
40.11
39.90
39.70
39.49
39.28
39.07
38.86
0.07
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppı

compound **20**

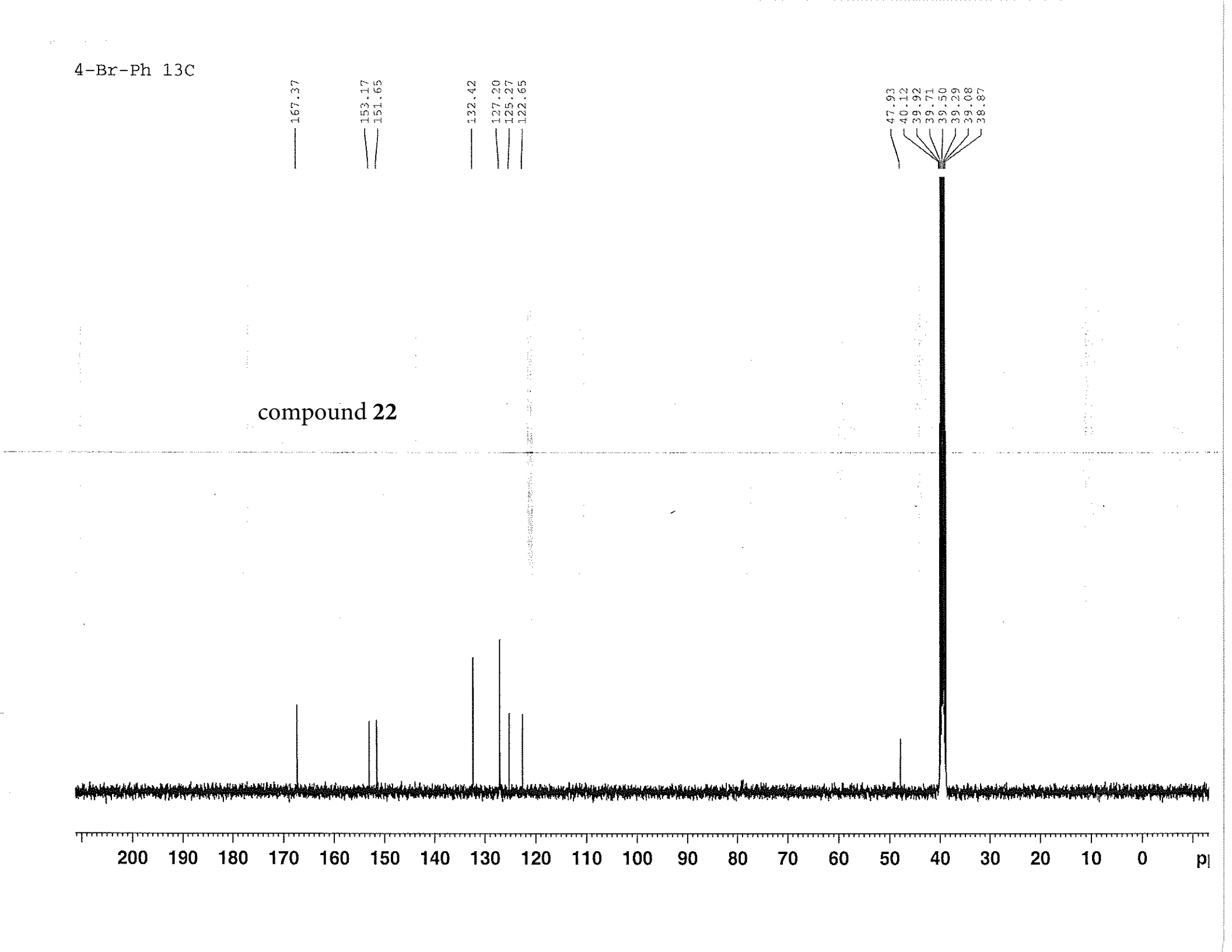

3-F-Ph
7.712
7.682
7.679
7.675
7.662
7.659
7.656
7.651
7.638
7.631
7.618
7.612
7.607
7.603
7.598
7.589
7.585
7.583
7.580
7.491
7.488
7.485
7.481
7.472
7.469
7.466
7.462
7.460
7.449
7.446
7.442
7.439
7.425
3.447
2.509
2.505
2.496
2.491
compound 21
10
9
8
7
6
5
4
3
2
1
0
ppı
0.90
3.13
2.01
2.00

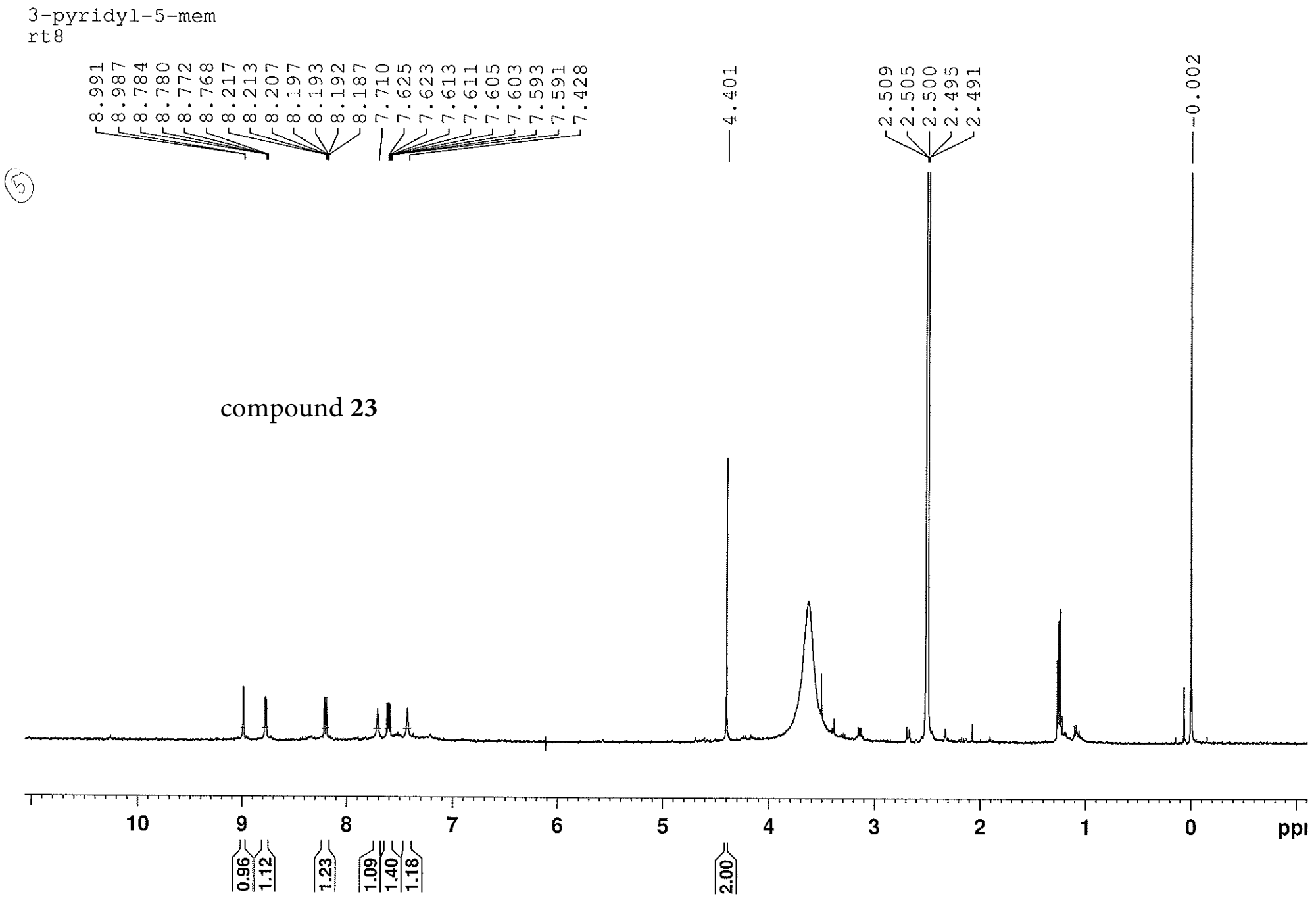

3-F-Ph
167.36
163.43
160.99
153.13
151.33
151.29
131.80
131.72
125.53
125.45
121.58
121.55
118.86
118.65
112.19
111.95
47.94
40.11
39.91
39.70
39.49
39.28
39.07
38.86
0.07
compound 21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

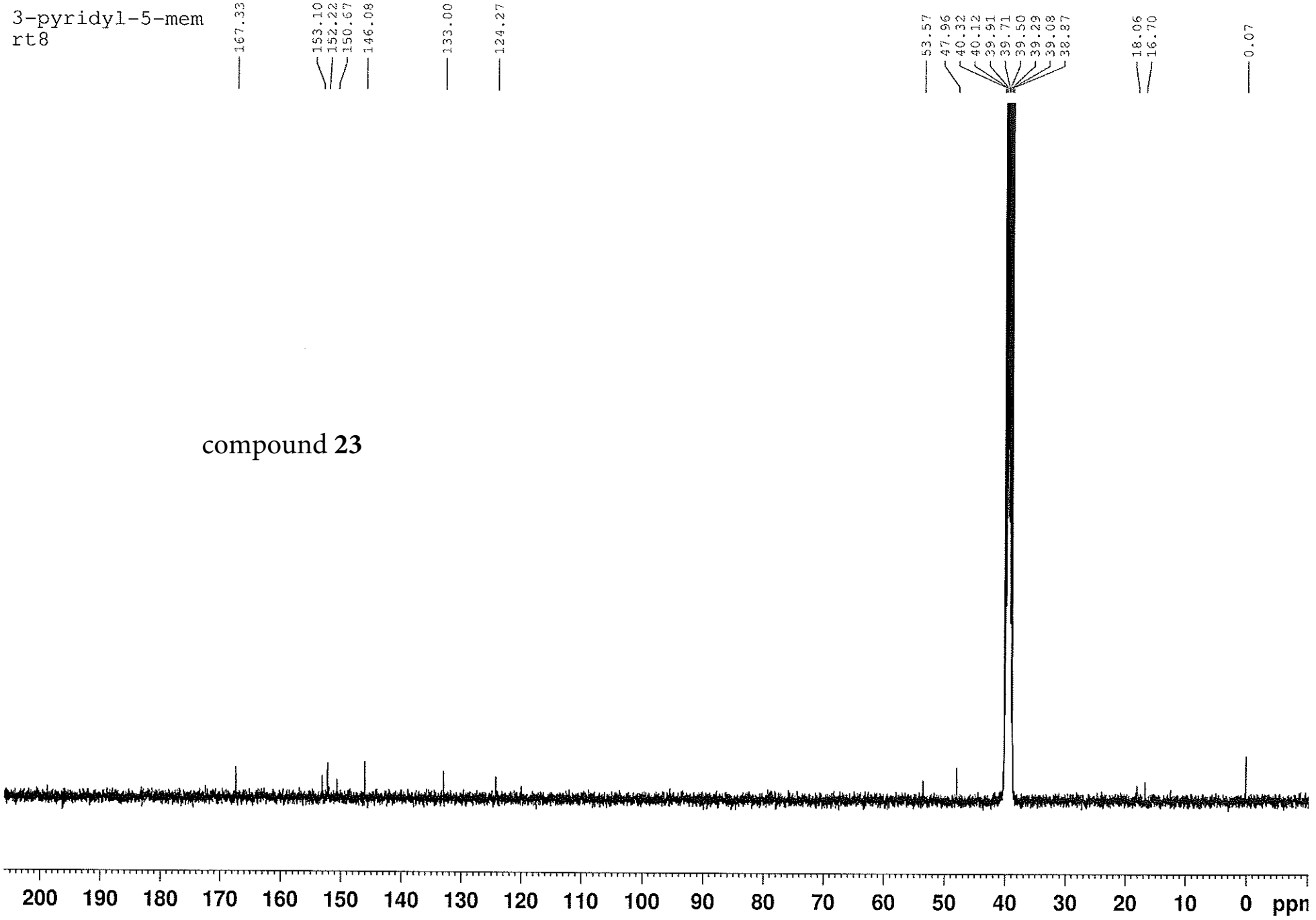
4-Br-Ph 1fter 18h



compound **22**

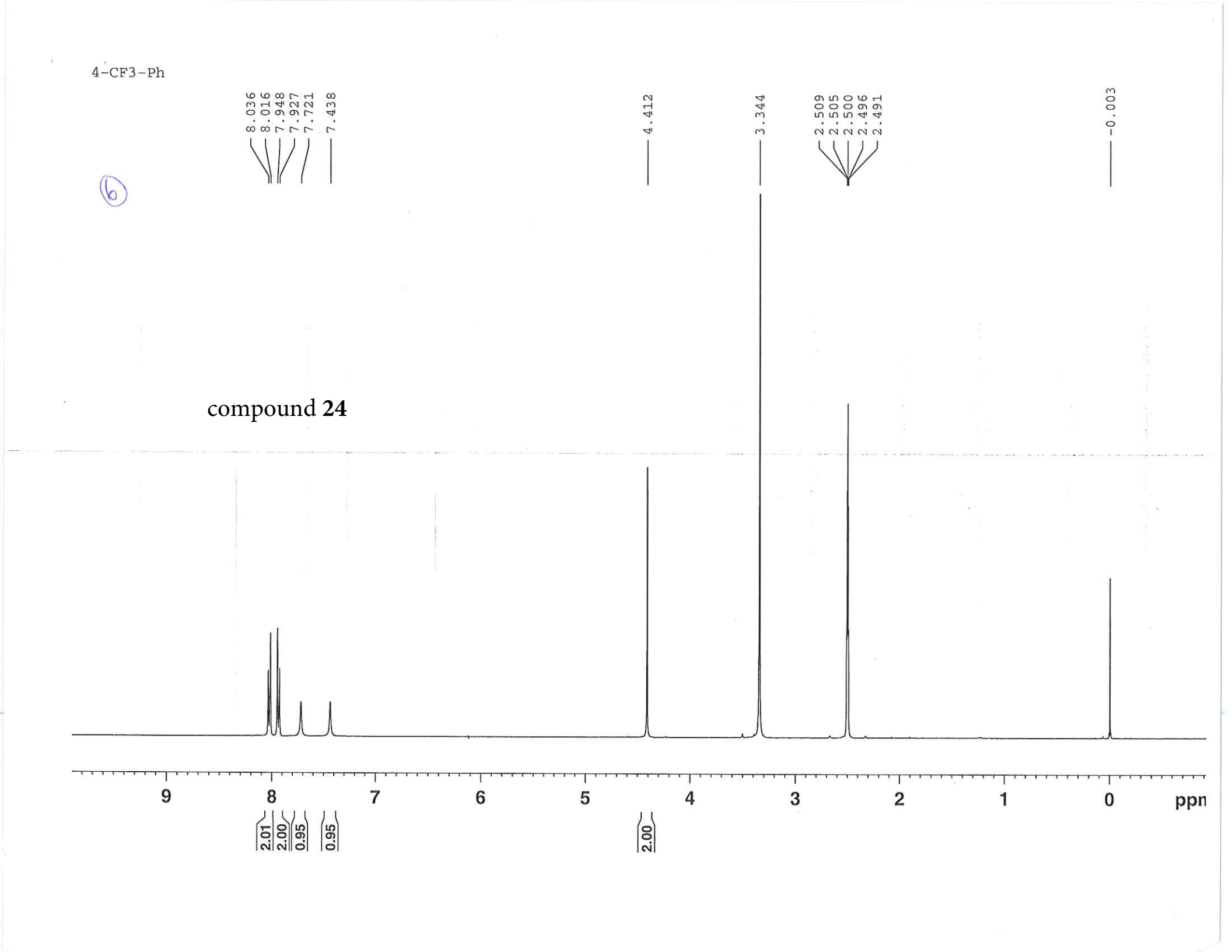

4-Br-Ph 13C
167.37
153.17
151.65
132.42
127.20
125.27
122.65
47.93
40.12
39.92
39.71
39.50
39.29
39.08
38.87
compound 22
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p


3-pyridyl-5-mem
rt8
8.991
8.987
8.784
8.780
8.772
8.768
8.217
8.213
8.207
8.197
8.193
8.192
8.187
7.710
7.625
7.623
7.613
7.611
7.605
7.603
7.593
7.591
7.428
4.401
2.509
2.505
2.500
2.495
2.491
0.002
compound 23
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.12
1.23
1.09
1.40
1.18
2.00

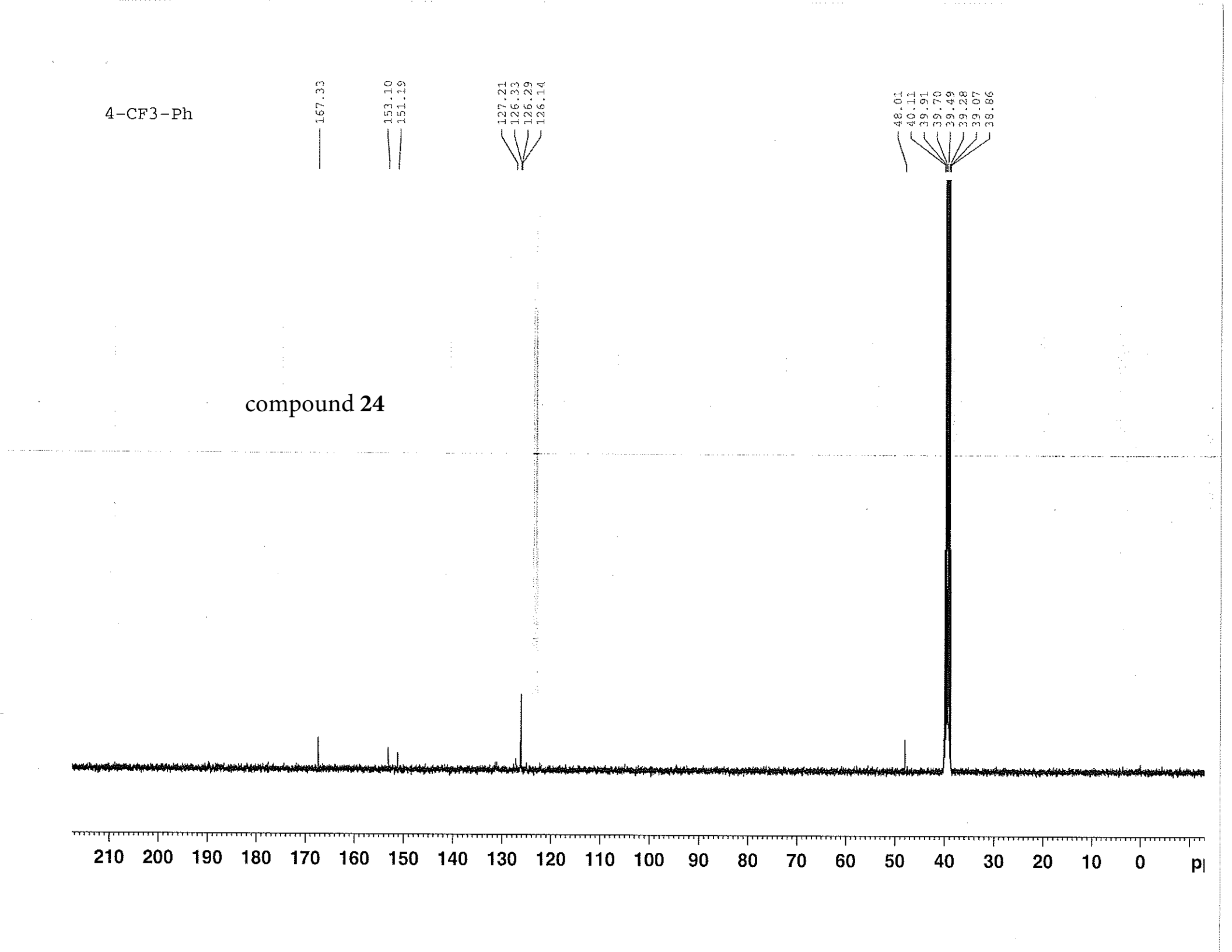

3-pyridyl-5-mem
rt8
167.33
153.10
152.22
150.67
146.08
133.00
124.27
53.57
47.96
40.32
40.12
39.91
39.71
39.50
39.29
39.08
38.87
18.06
16.70
0.07
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

compound **23**

4-CF3-Ph



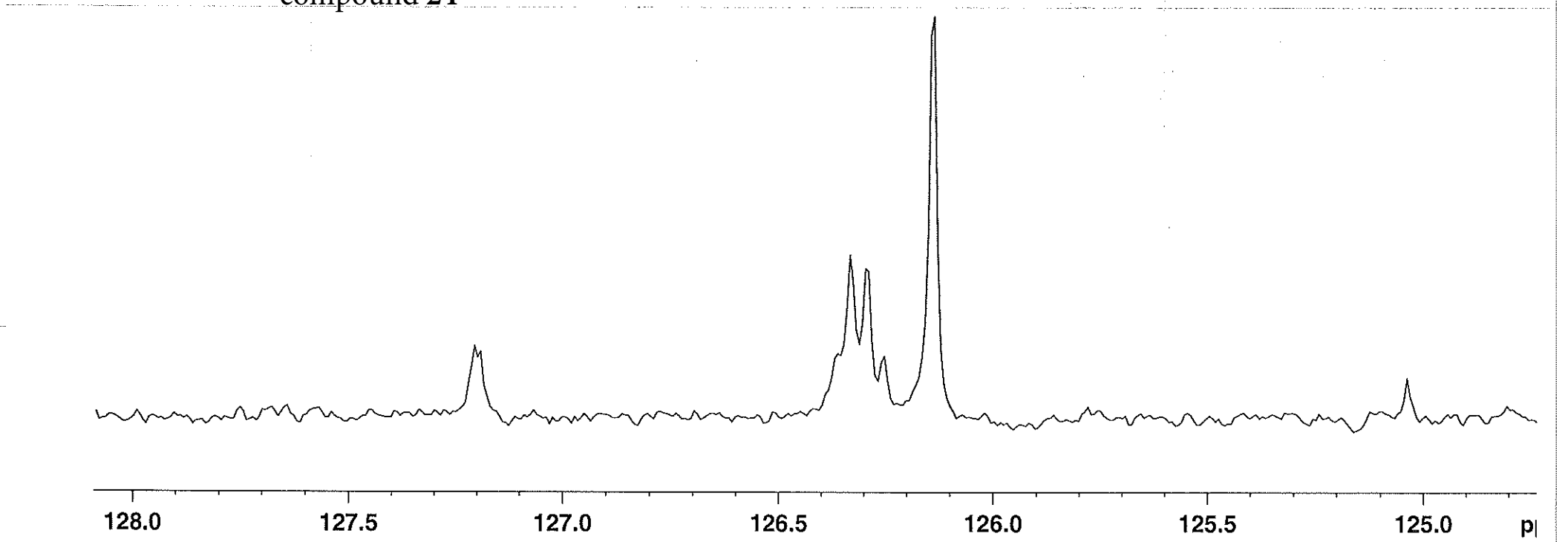
compound **24**

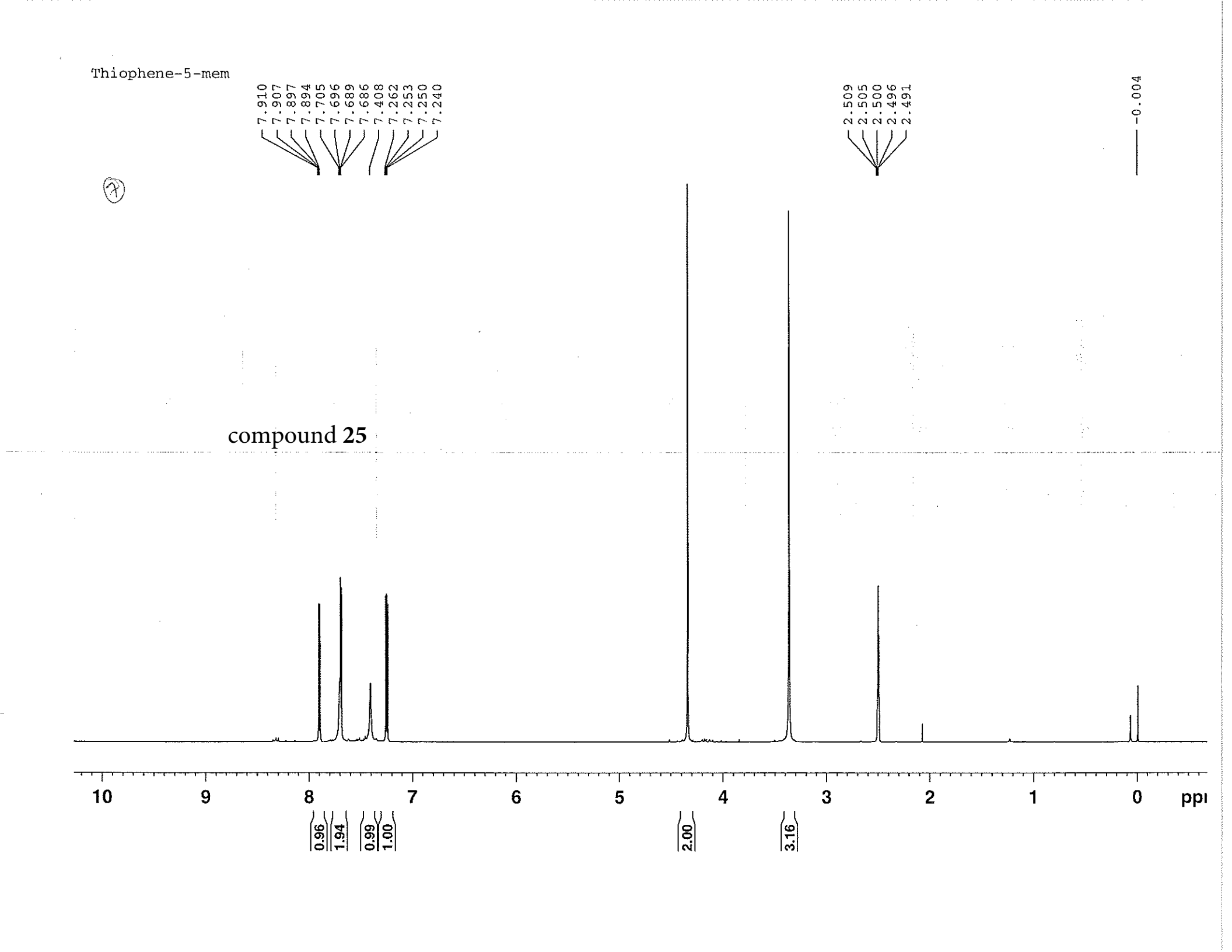

4-CF3-Ph
167.33
153.10
151.19
127.21
126.33
126.29
126.14
48.01
40.11
39.91
39.70
39.49
39.28
39.07
38.86
compound 24
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p

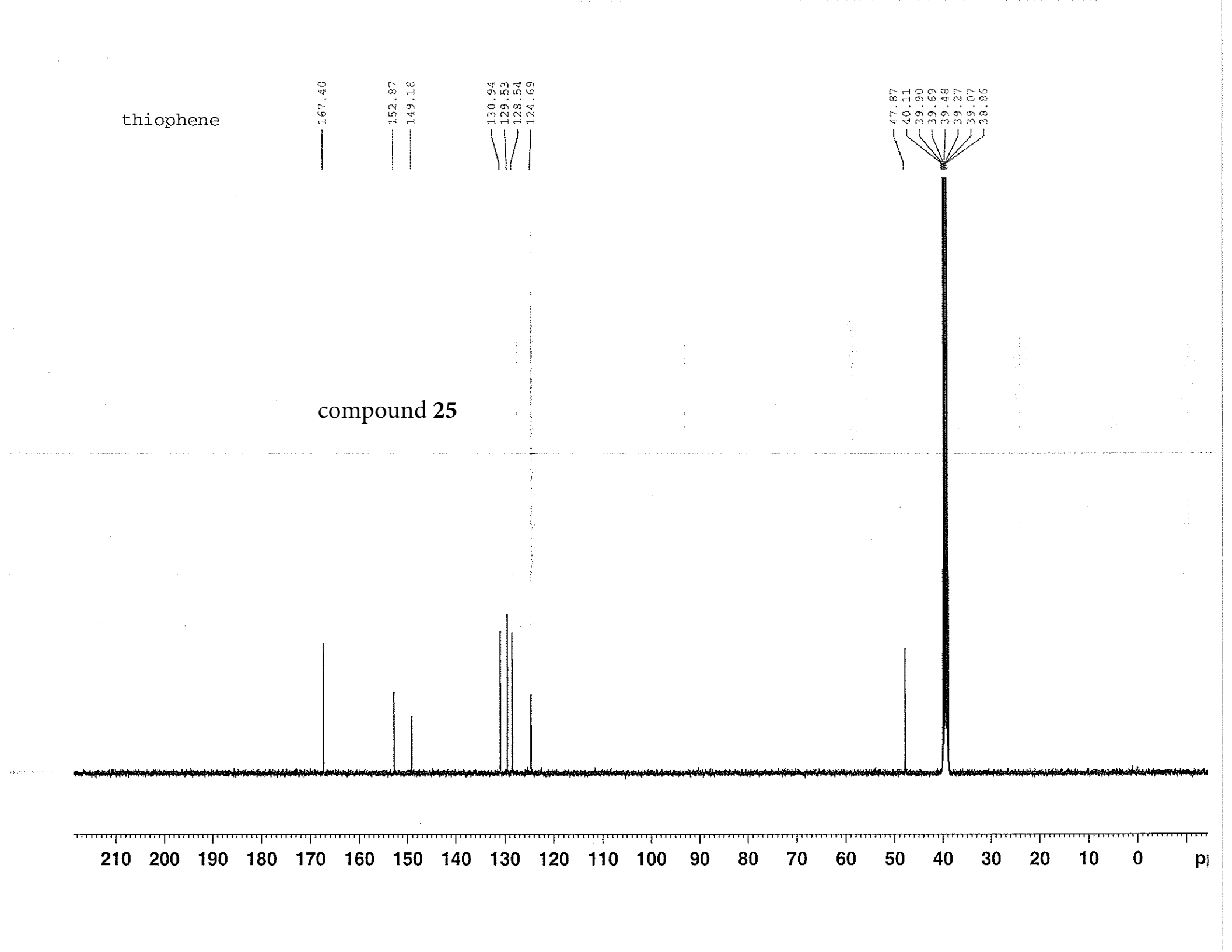
4-CF3-Ph

127.21
126.33
126.30
126.26
126.14
125.04

compound **24**




Thiophene-5-mem
7.910
7.907
7.897
7.894
7.705
7.696
7.689
7.686
7.408
7.262
7.253
7.250
7.240
2.509
2.505
2.500
2.496
2.491
-0.004
compound 25
10
9
8
7
6
5
4
3
2
1
0
ppı
0.96
1.94
0.99
1.00
2.00
3.16


thiophene
167.40
152.87
149.18
130.94
129.53
128.54
124.69
47.87
40.11
39.90
39.69
39.48
39.27
39.07
38.86
compound 25
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p

4-Cl-Ph-comp8

7.840
7.834
7.829
7.817
7.812
7.806
7.713
7.657
7.651
7.646
7.634
7.629
7.622
7.425

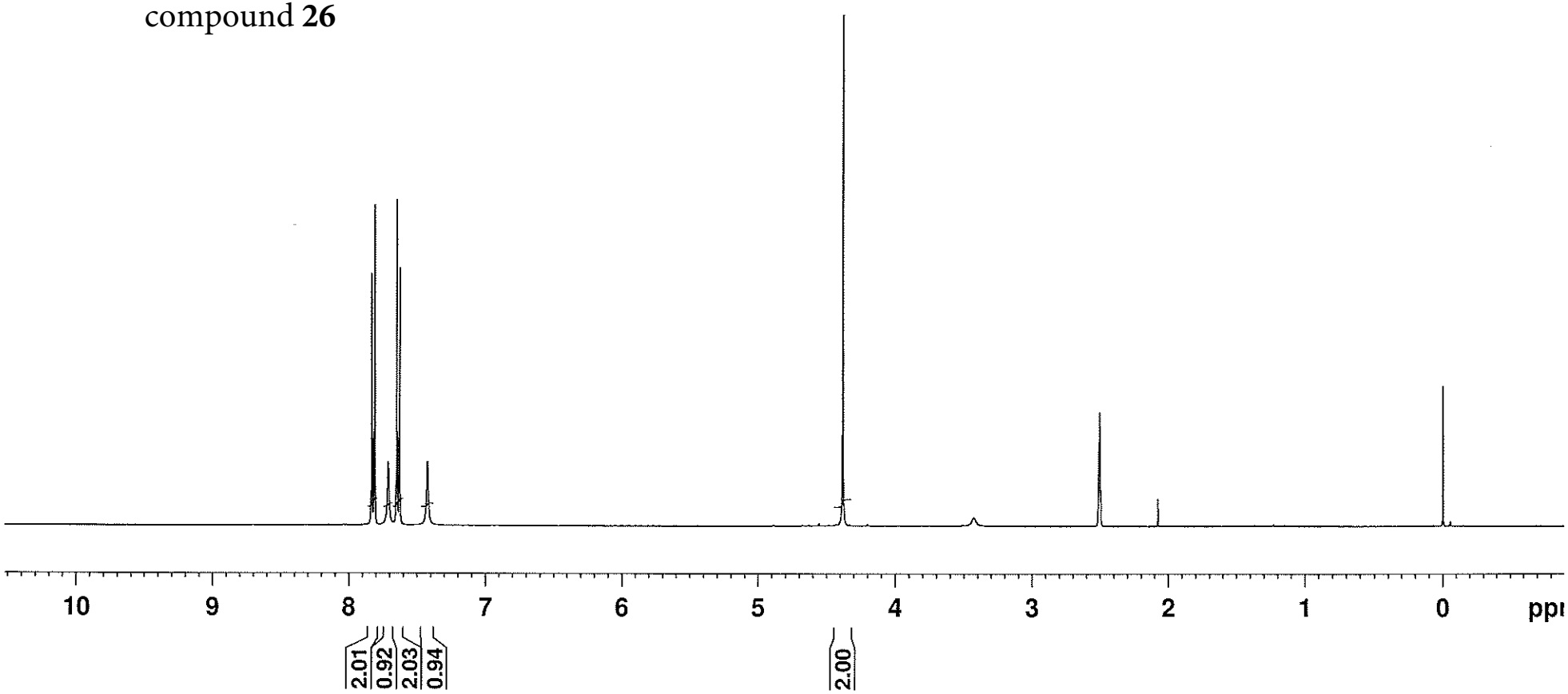
4.383

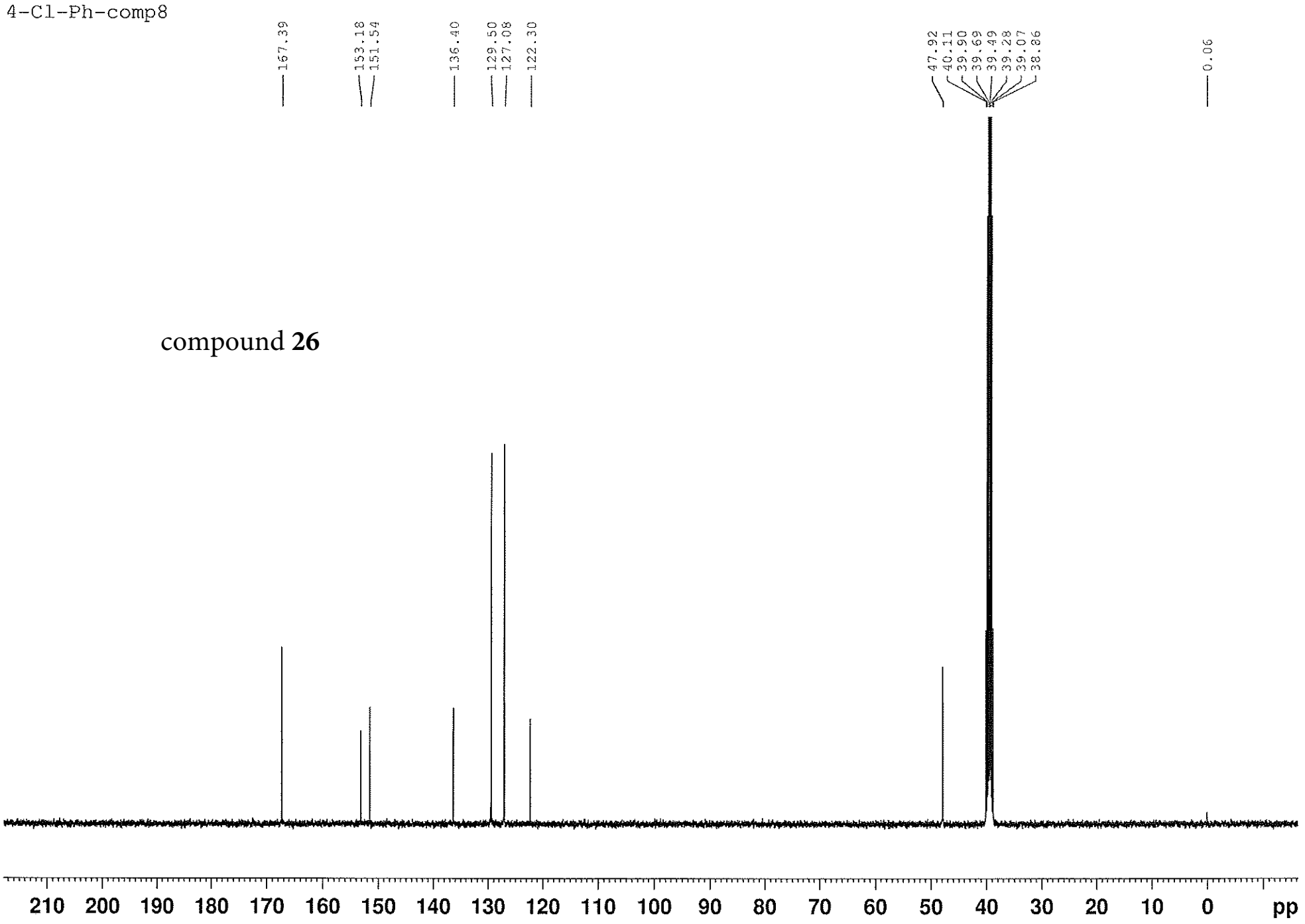
2.515
2.511
2.506
2.502
2.497
2.079

0.000

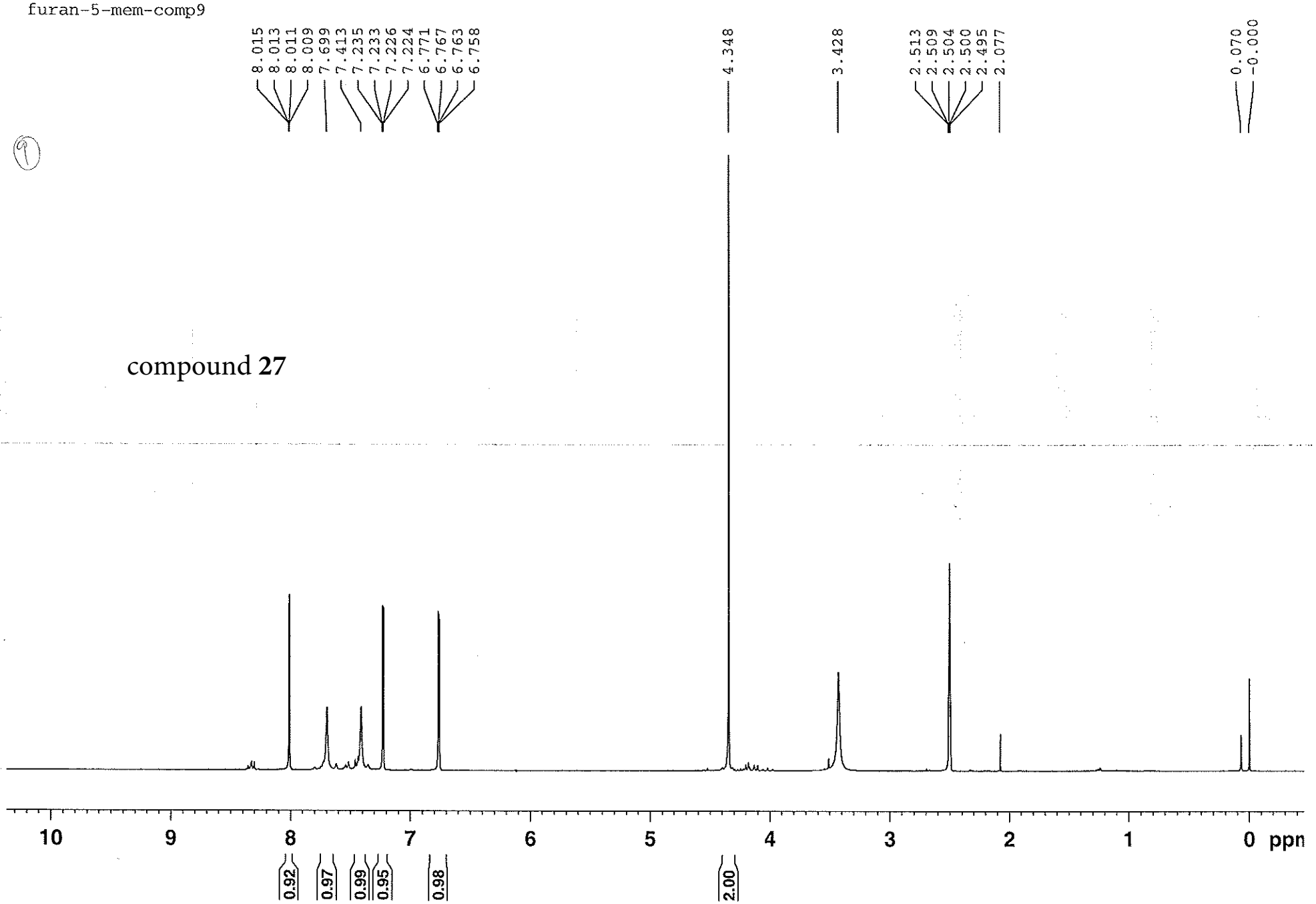
(8)

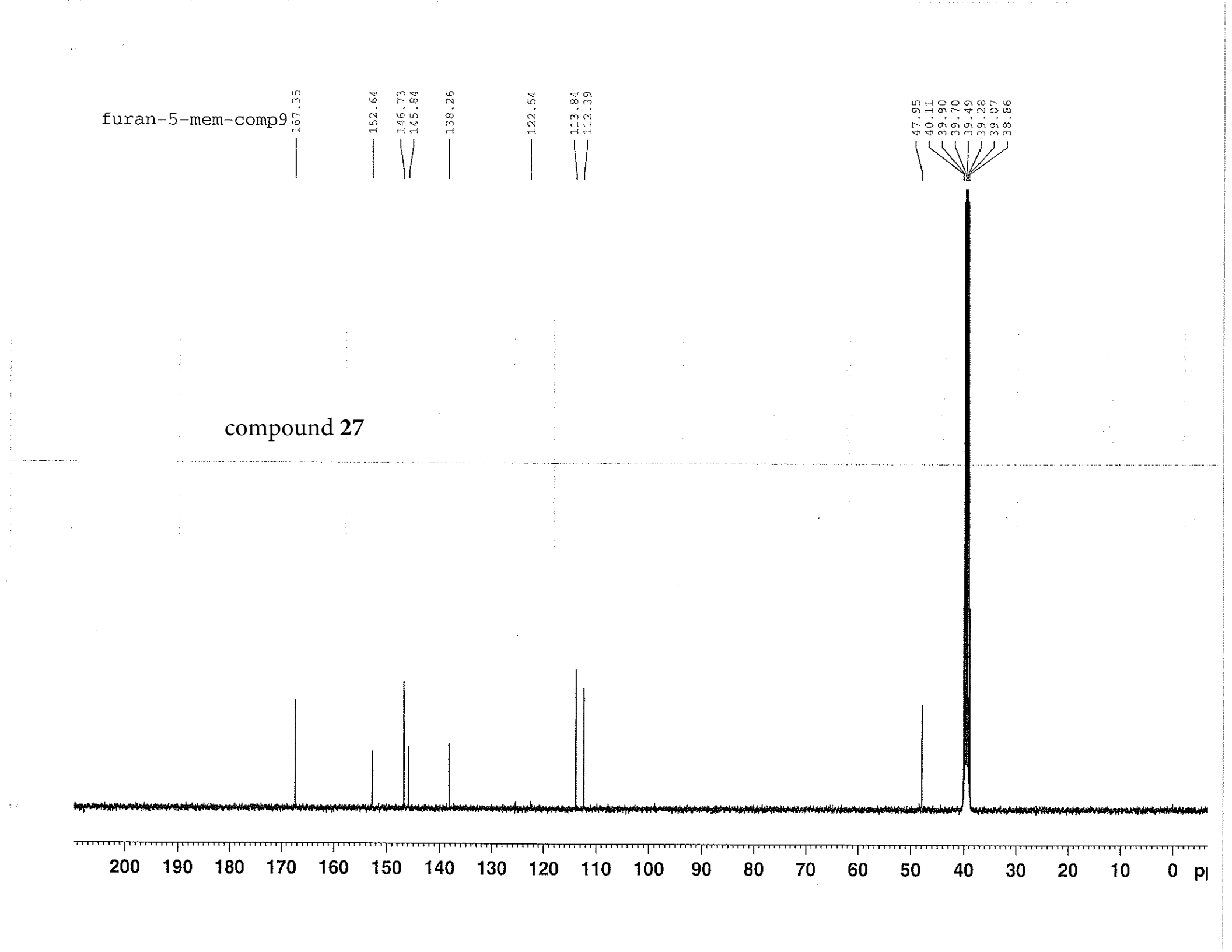
compound **26**




4-Cl-Ph-comp8
167.39
153.18
151.54
136.40
129.50
127.08
122.30
47.92
40.11
39.90
39.69
39.49
39.28
39.07
38.86
0.06
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

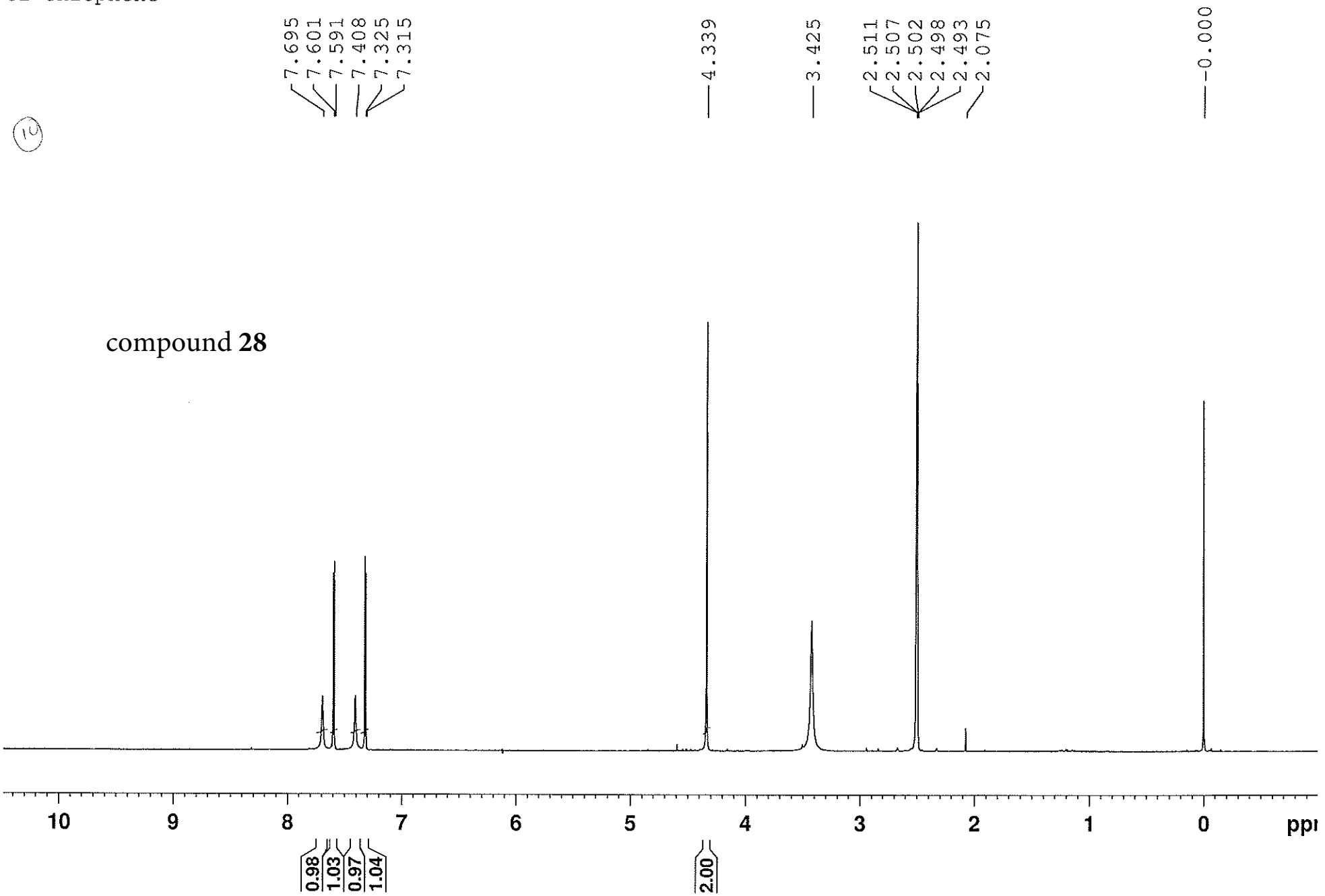
compound **26**

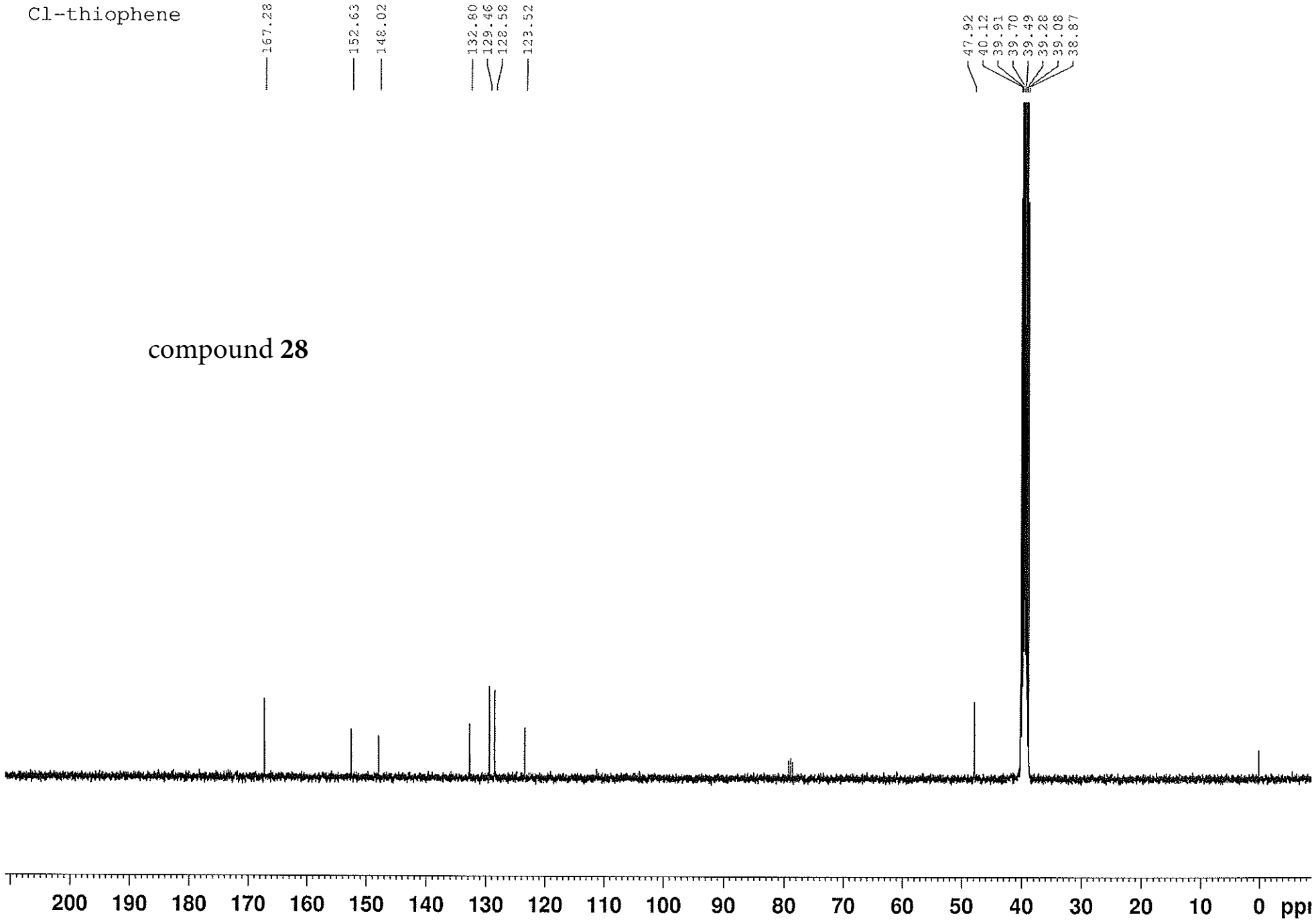

furan-5-mem-comp9
8.015
8.013
8.011
8.009
7.699
7.413
7.235
7.233
7.226
7.224
6.771
6.767
6.763
6.758
4.348
3.428
2.513
2.509
2.504
2.500
2.495
2.077
0.070
-0.000
9
compound 27
10
9
8
7
6
5
4
3
2
1
0
ppm
0.92
0.97
0.99
0.95
0.98
2.00


furan-5-mem-comp9
167.35
152.64
146.73
145.84
138.26
122.54
113.84
112.39
47.95
40.11
39.90
39.70
39.49
39.28
39.07
38.86
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p

compound **27**

Cl-thiophene



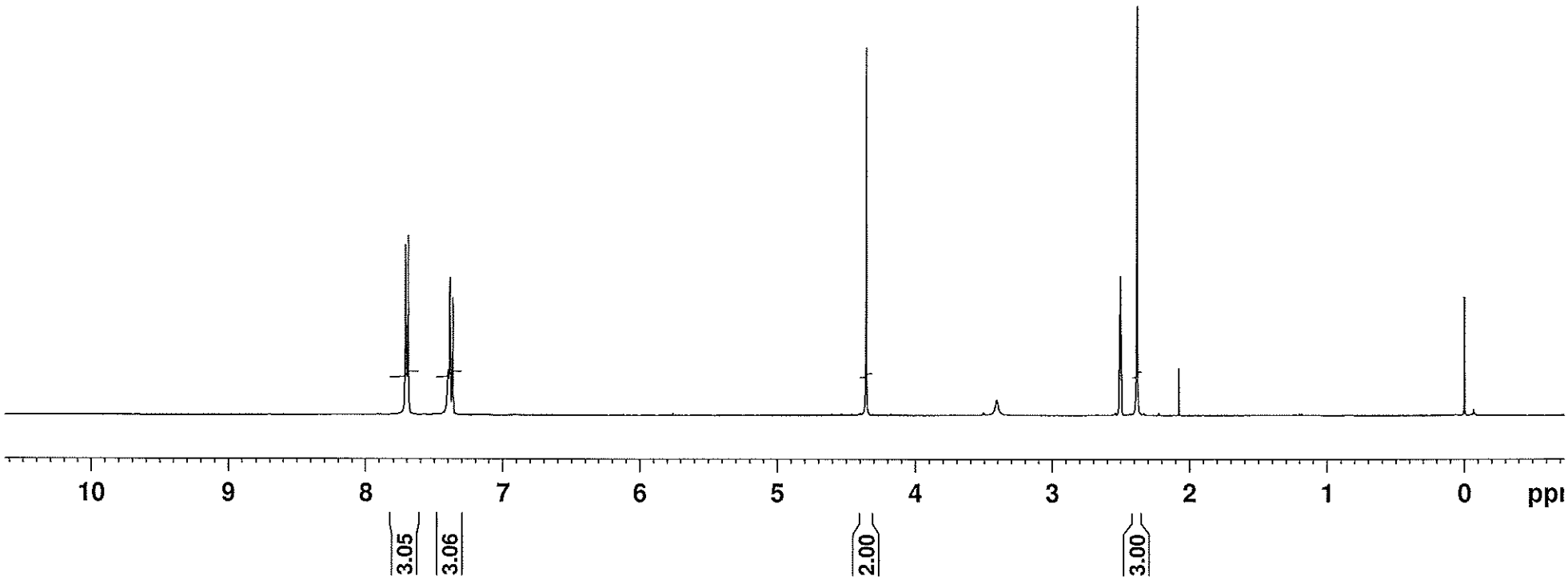

Cl-thiophene
167.28
152.63
148.02
132.80
129.46
128.58
123.52
47.92
40.12
39.91
39.70
39.49
39.28
39.08
38.87
compound 28
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

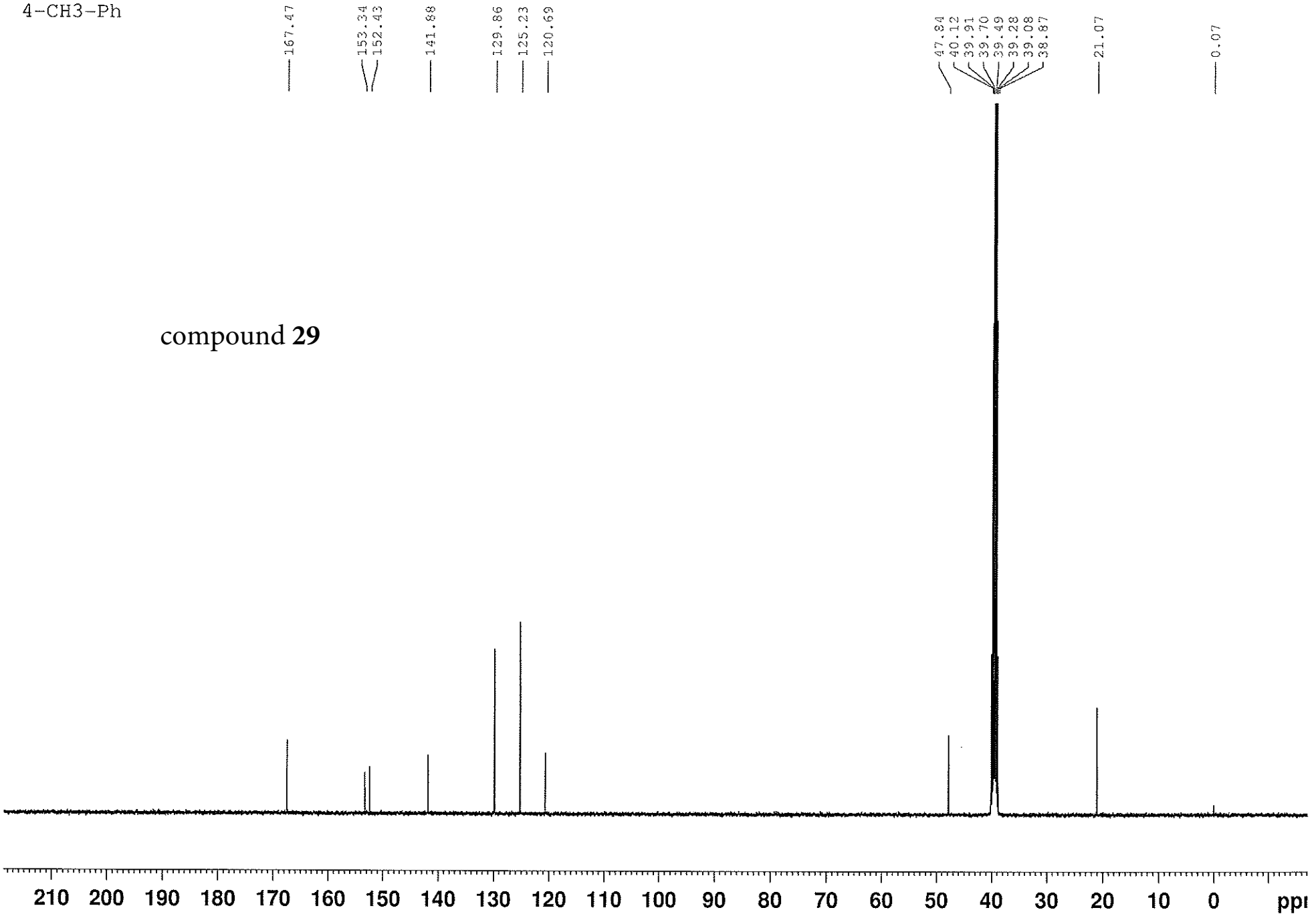
4-CH3-Ph

(12)

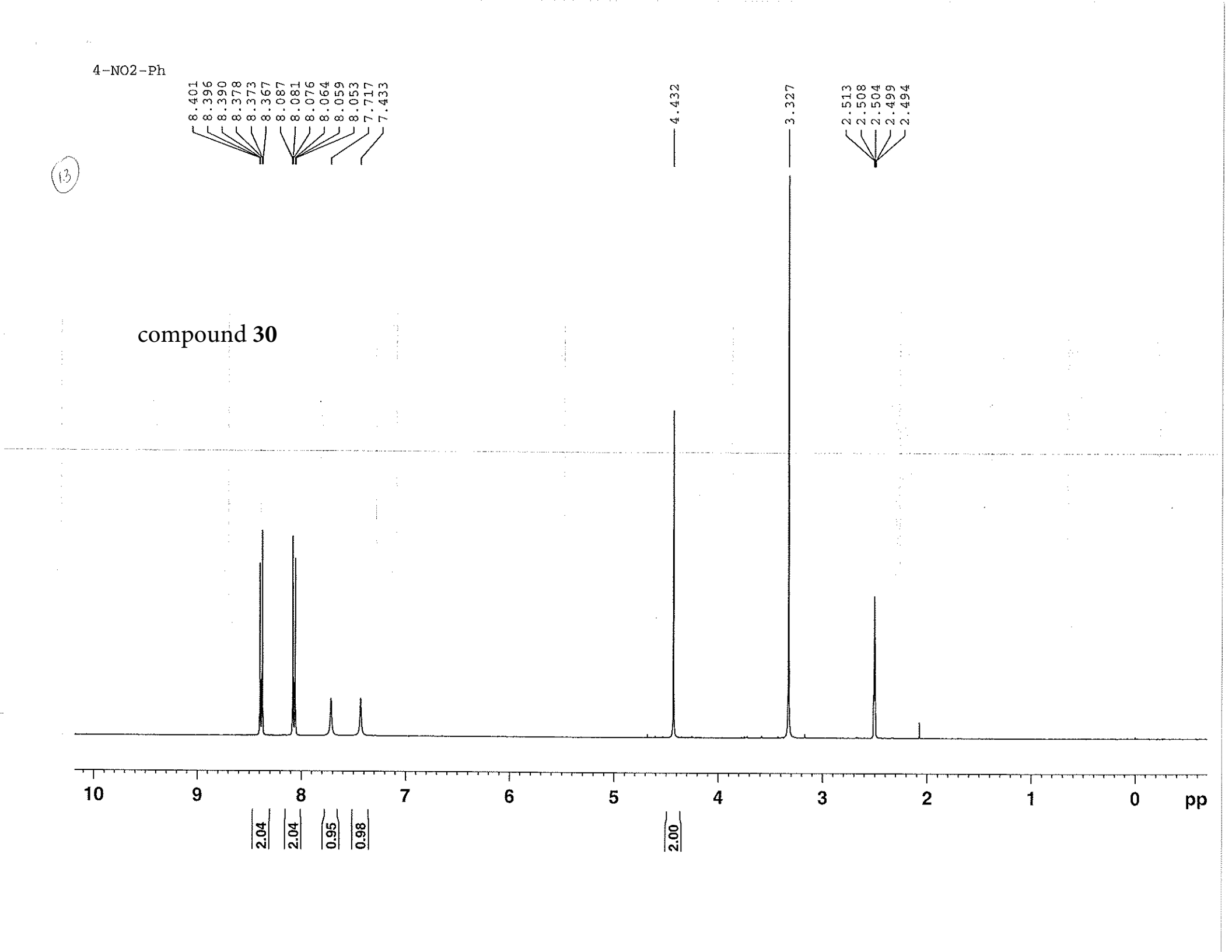
7.712
7.708
7.696
7.691
7.400
7.386
7.367
4.358
3.409
2.512
2.508
2.503
2.499
2.494
2.383
2.076
0.000

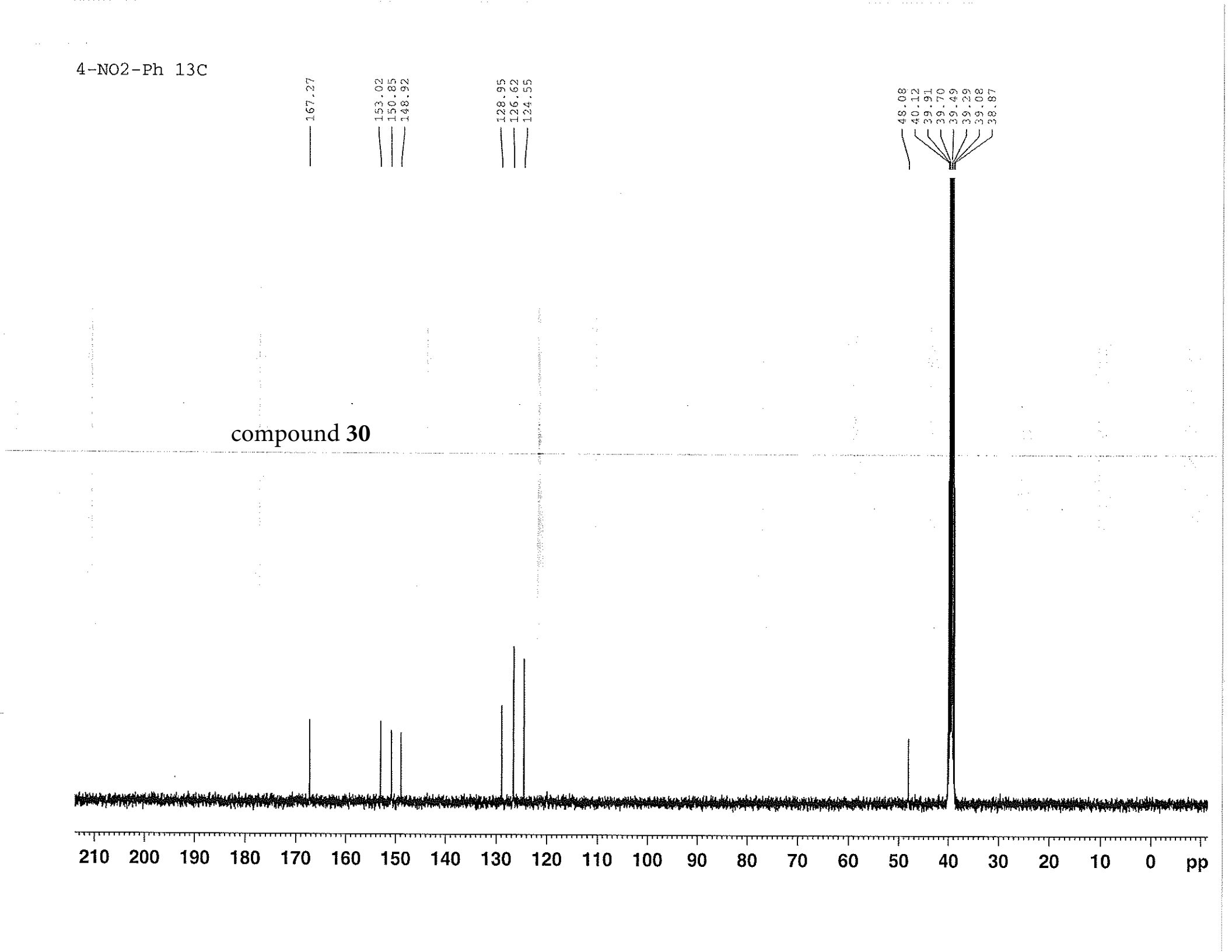
compound **29**




4-CH3-Ph
167.47
153.34
152.43
141.88
129.86
125.23
120.69
47.84
40.12
39.91
39.70
39.49
39.28
39.08
38.87
21.07
0.07
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

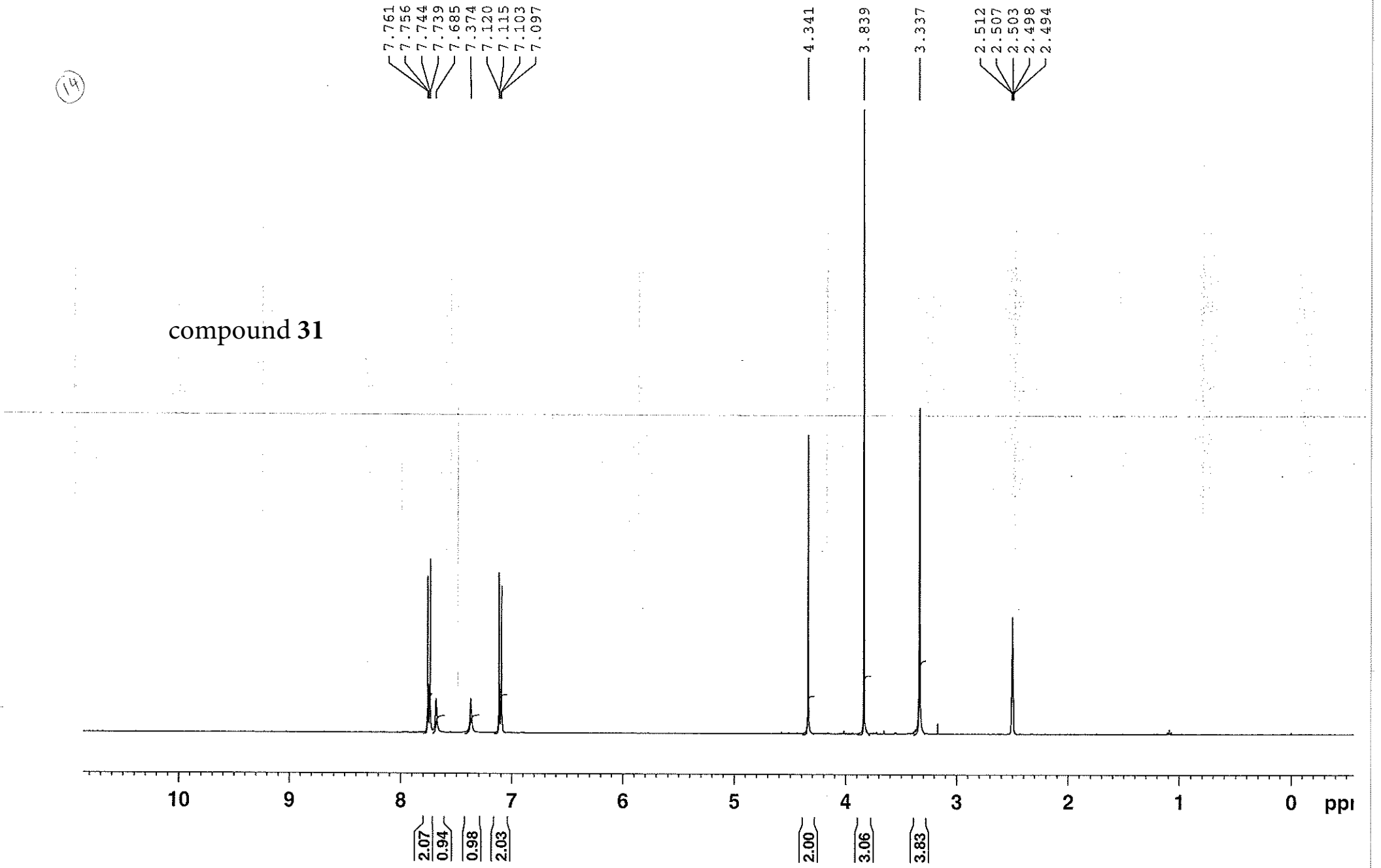
compound **29**


4-NO2-Ph
8.401
8.396
8.390
8.378
8.373
8.367
8.087
8.081
8.076
8.064
8.059
8.053
7.717
7.433
4.432
3.327
2.513
2.508
2.504
2.499
2.494
(13)
compound 30
10
9
8
7
6
5
4
3
2
1
0
pp
2.04
2.04
0.95
0.98
2.00

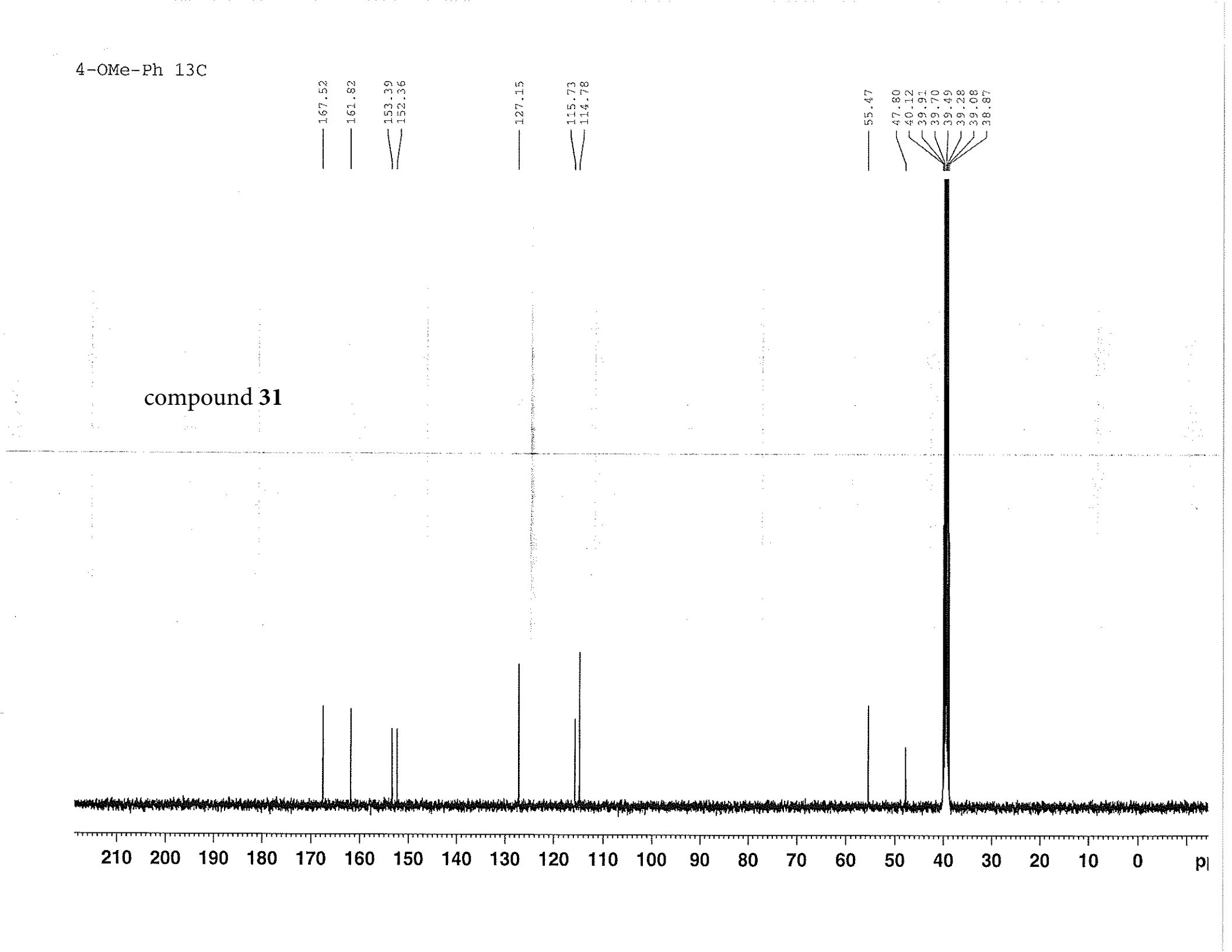

4-NO2-Ph 13C
167.27
153.02
150.85
148.92
128.95
126.62
124.55
48.08
40.12
39.91
39.70
39.49
39.29
39.08
38.87
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

compound **30**

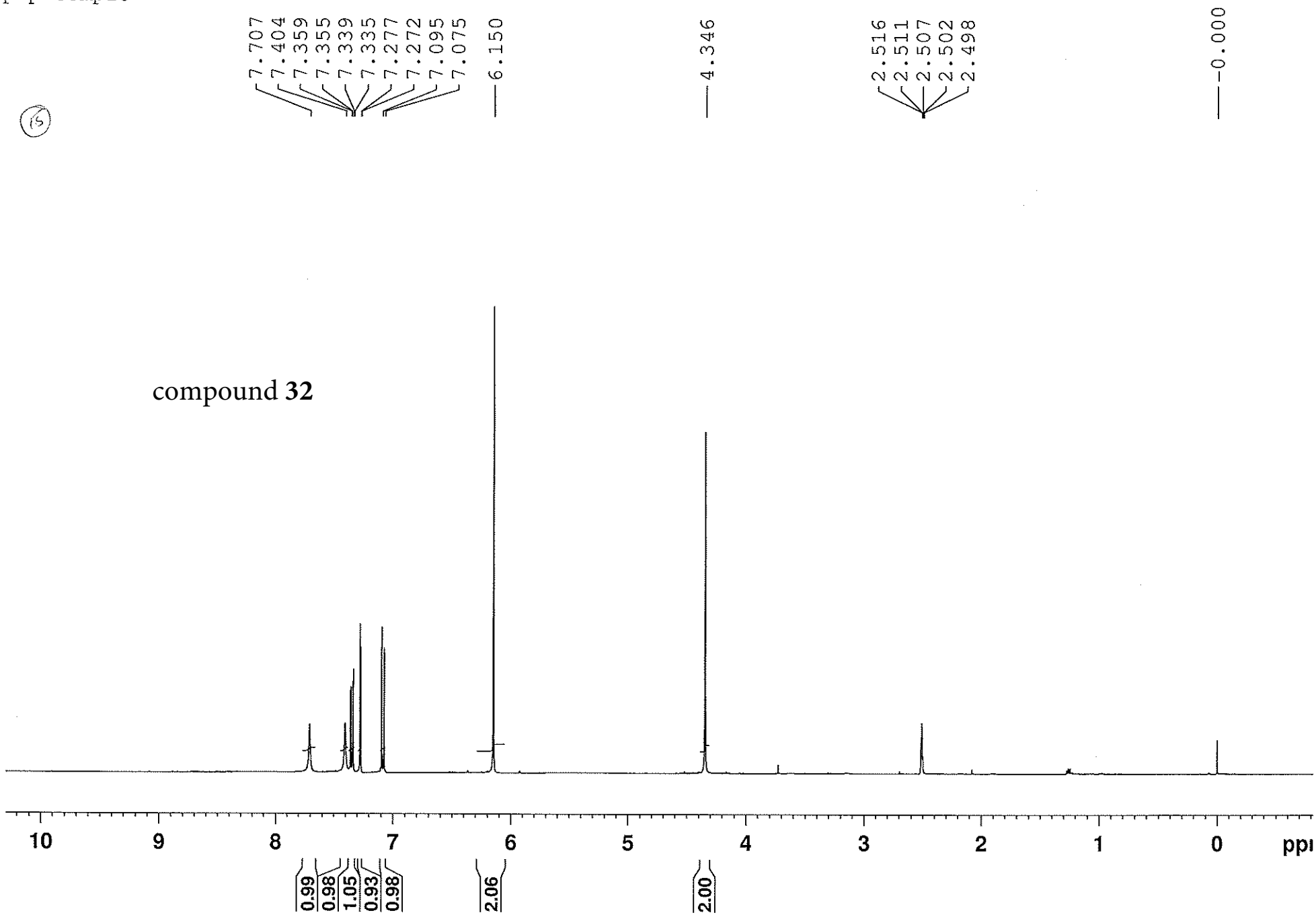
4-OMe-Ph

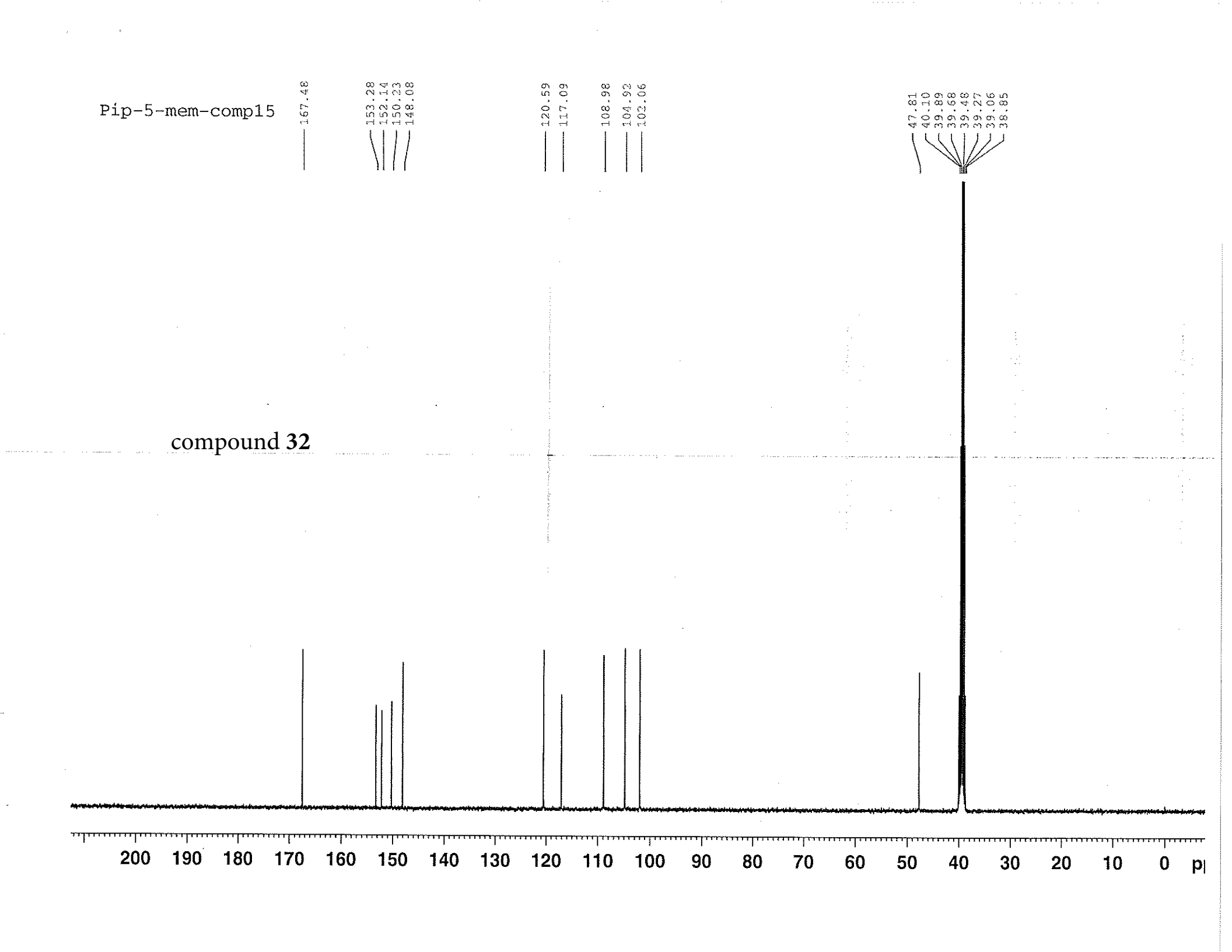


compound **31**


4-OMe-Ph 13C
167.52
161.82
153.39
152.36
127.15
115.73
114.78
55.47
47.80
40.12
39.91
39.70
39.49
39.28
39.08
38.87
compound 31
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p

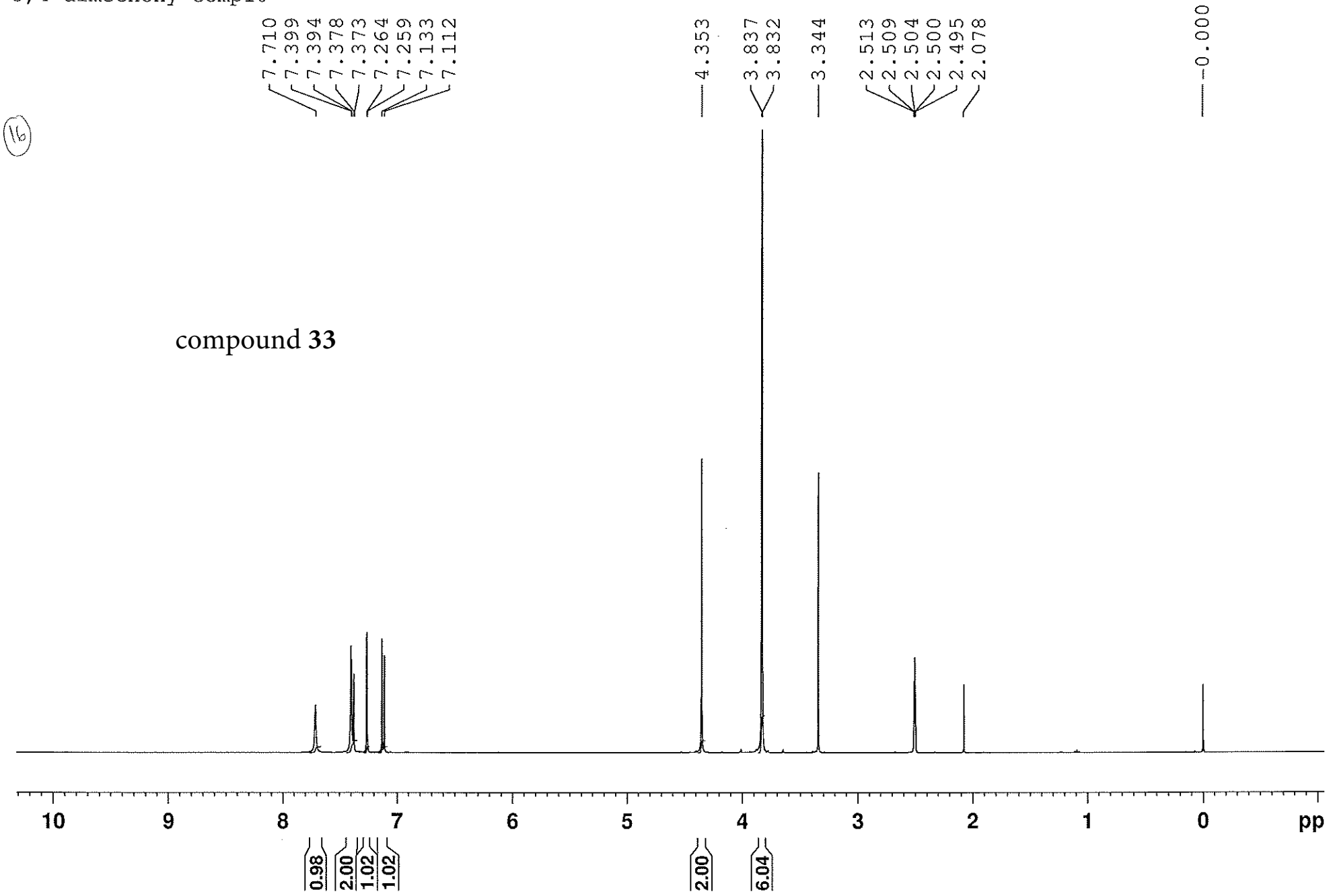
pip-comp15


7.707
7.404
7.359
7.355
7.339
7.335
7.277
7.272
7.095
7.075
6.150
4.346
2.516
2.511
2.507
2.502
2.498
0.000
compound 32
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
0.98
1.05
0.93
0.98
2.06
2.00


Pip-5-mem-comp15
167.48
153.28
152.14
150.23
148.08
120.59
117.09
108.98
104.92
102.06
47.81
40.10
39.89
39.68
39.48
39.27
39.06
38.85
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
p

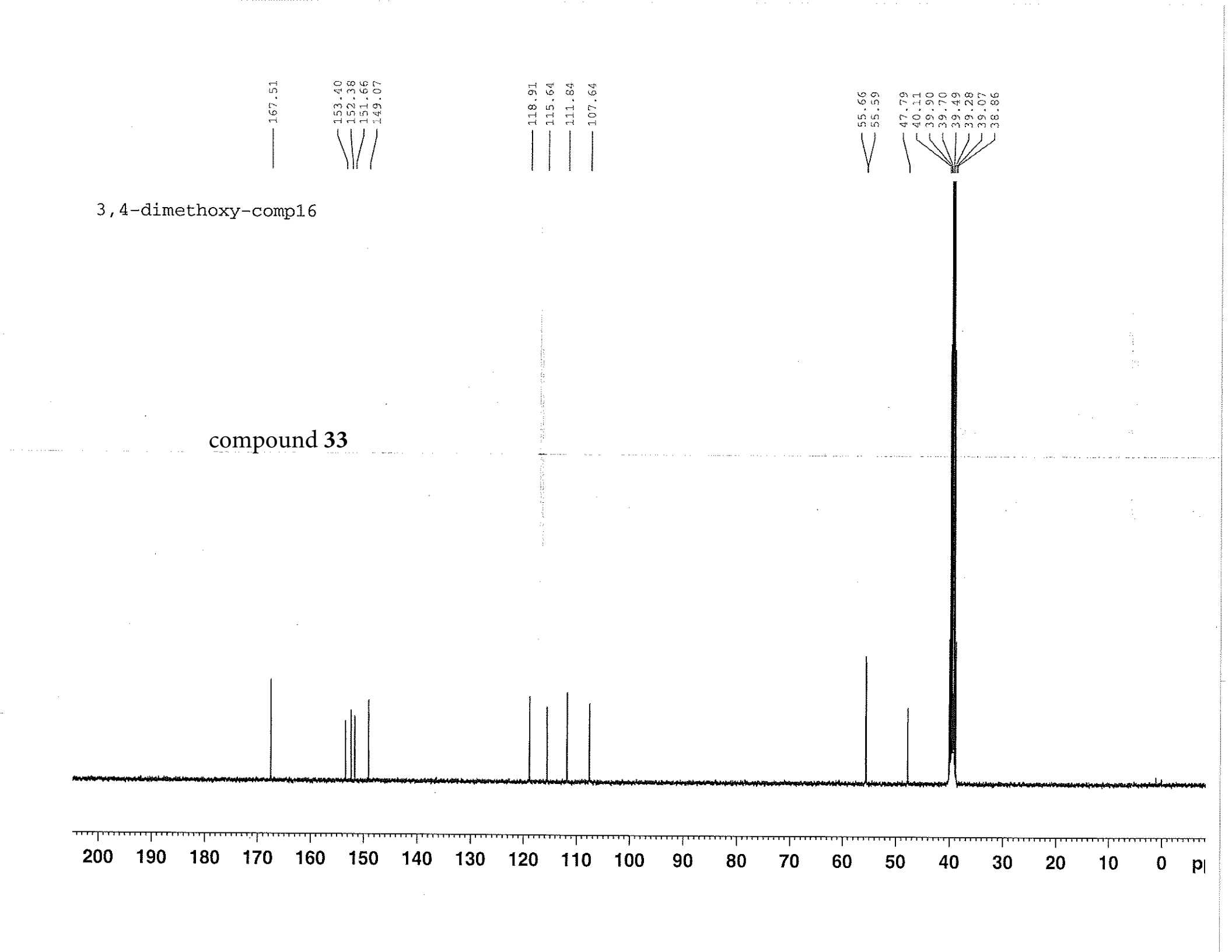
compound **32**

3,4-dimethoxy-comp16

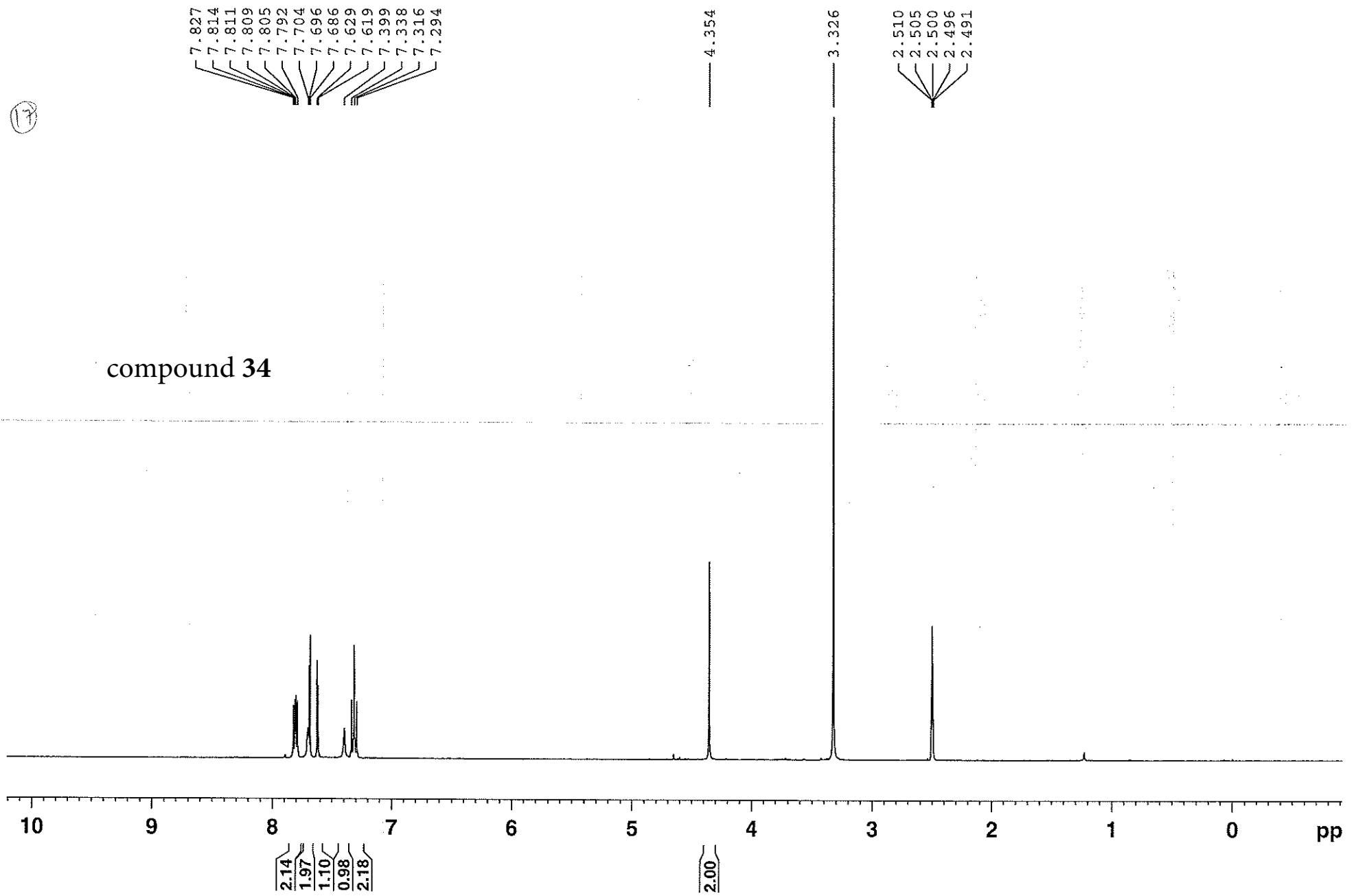


(16)

compound **33**

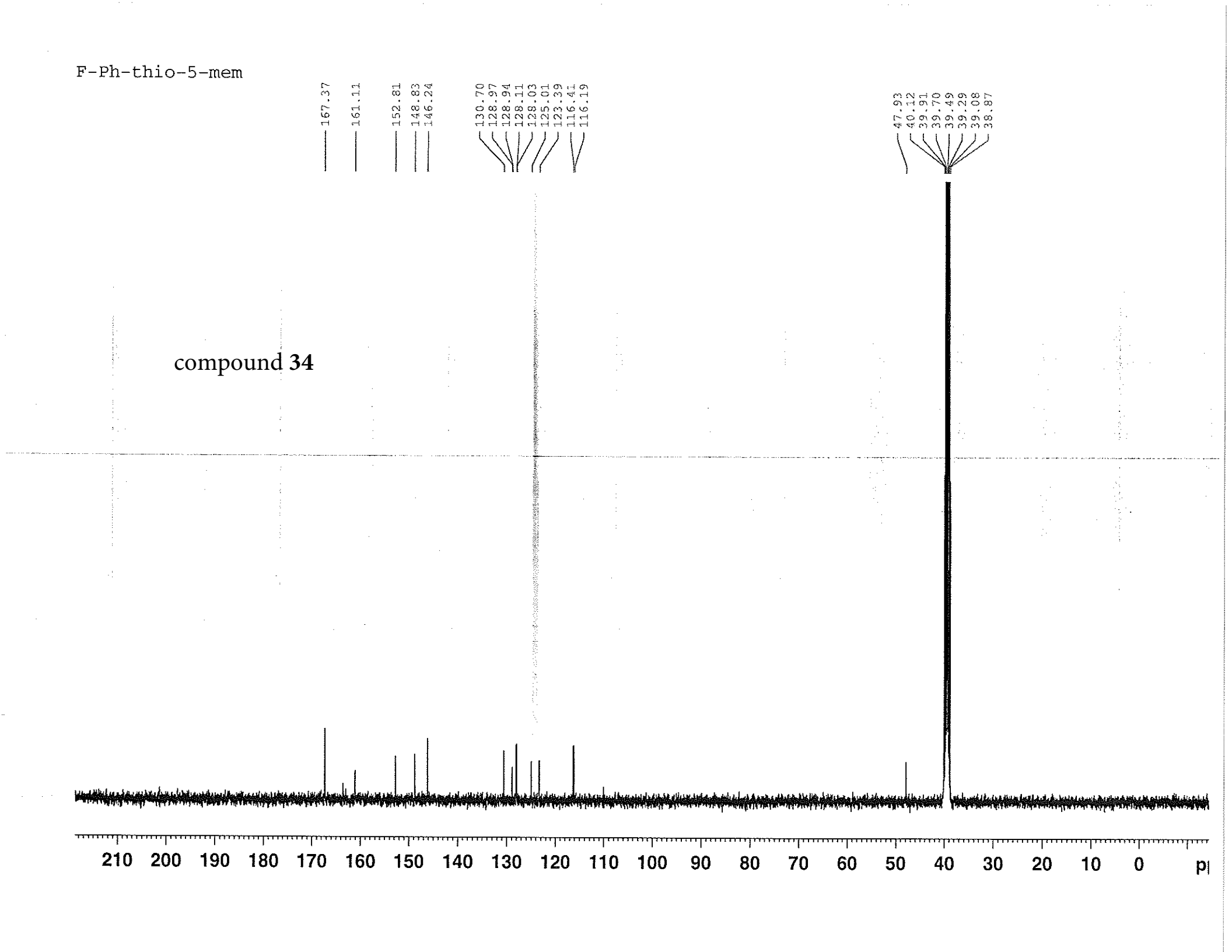

167.51
153.40
152.38
151.66
149.07
118.91
115.64
111.84
107.64
55.66
55.59
47.79
40.11
39.90
39.70
39.49
39.28
39.07
38.86
3,4-dimethoxy-comp16
compound 33
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 p

F-Ph-thio-5-mem



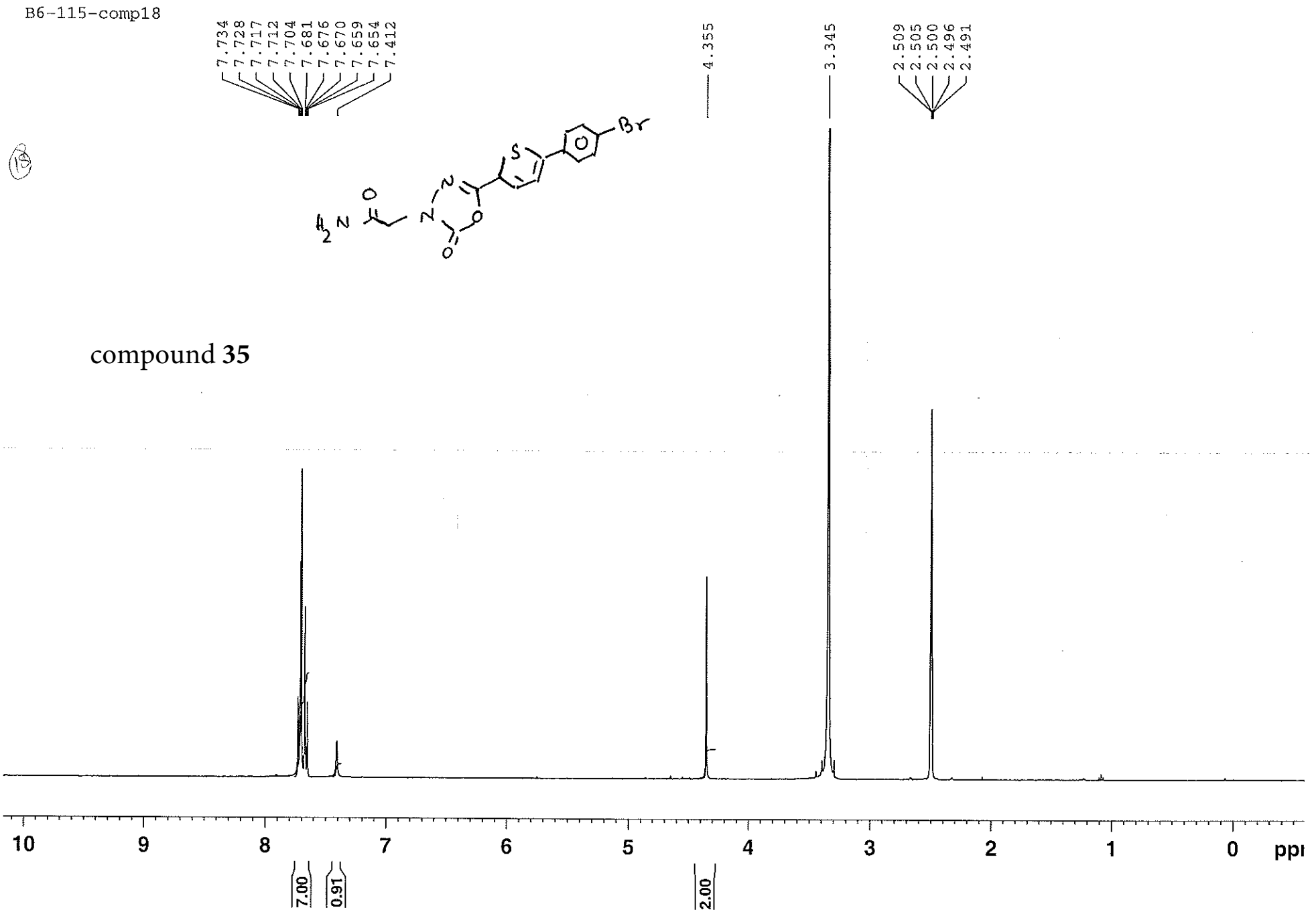
compound **34**

F-Ph-thio-5-mem



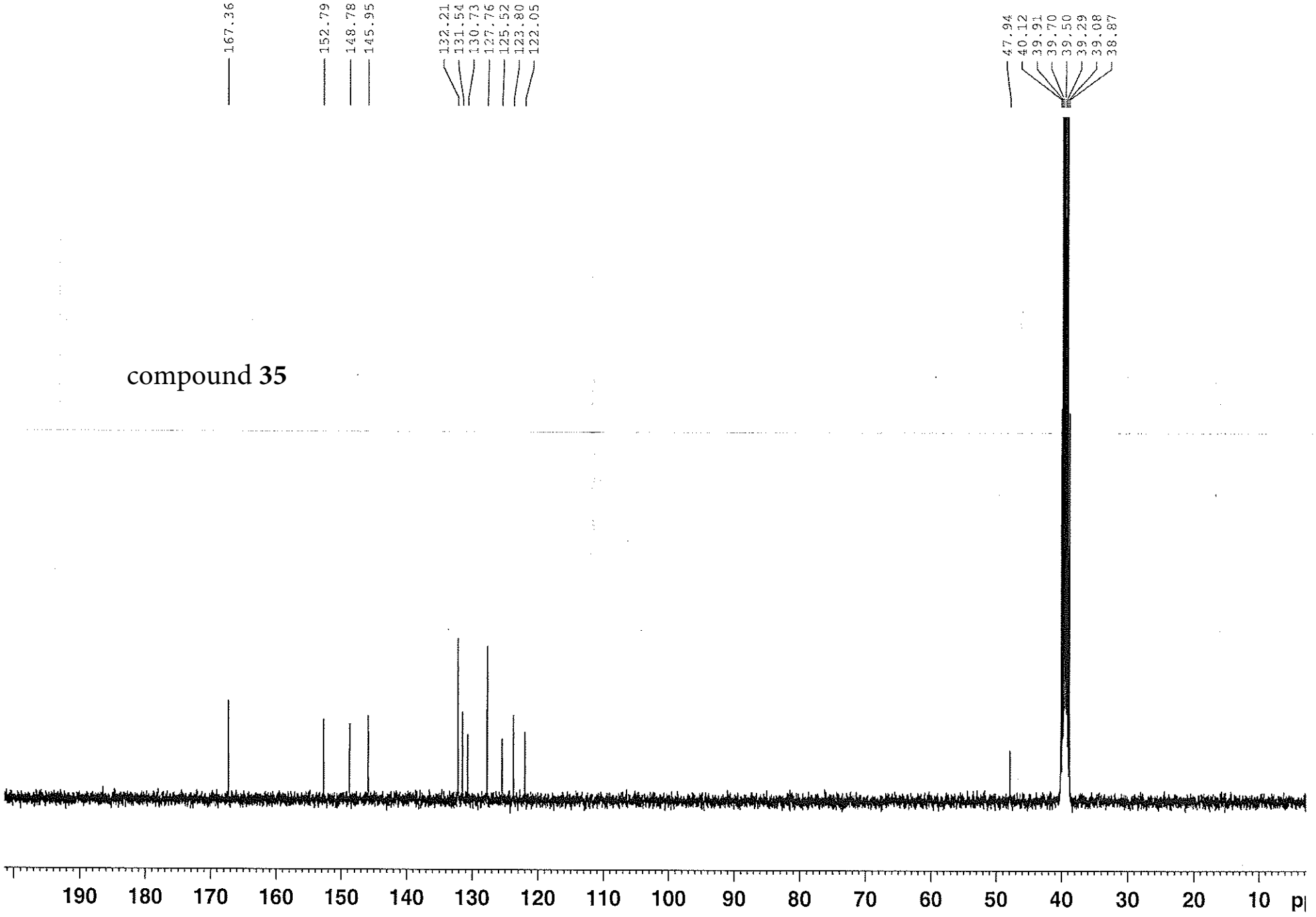
compound **34**

B6-115-comp18



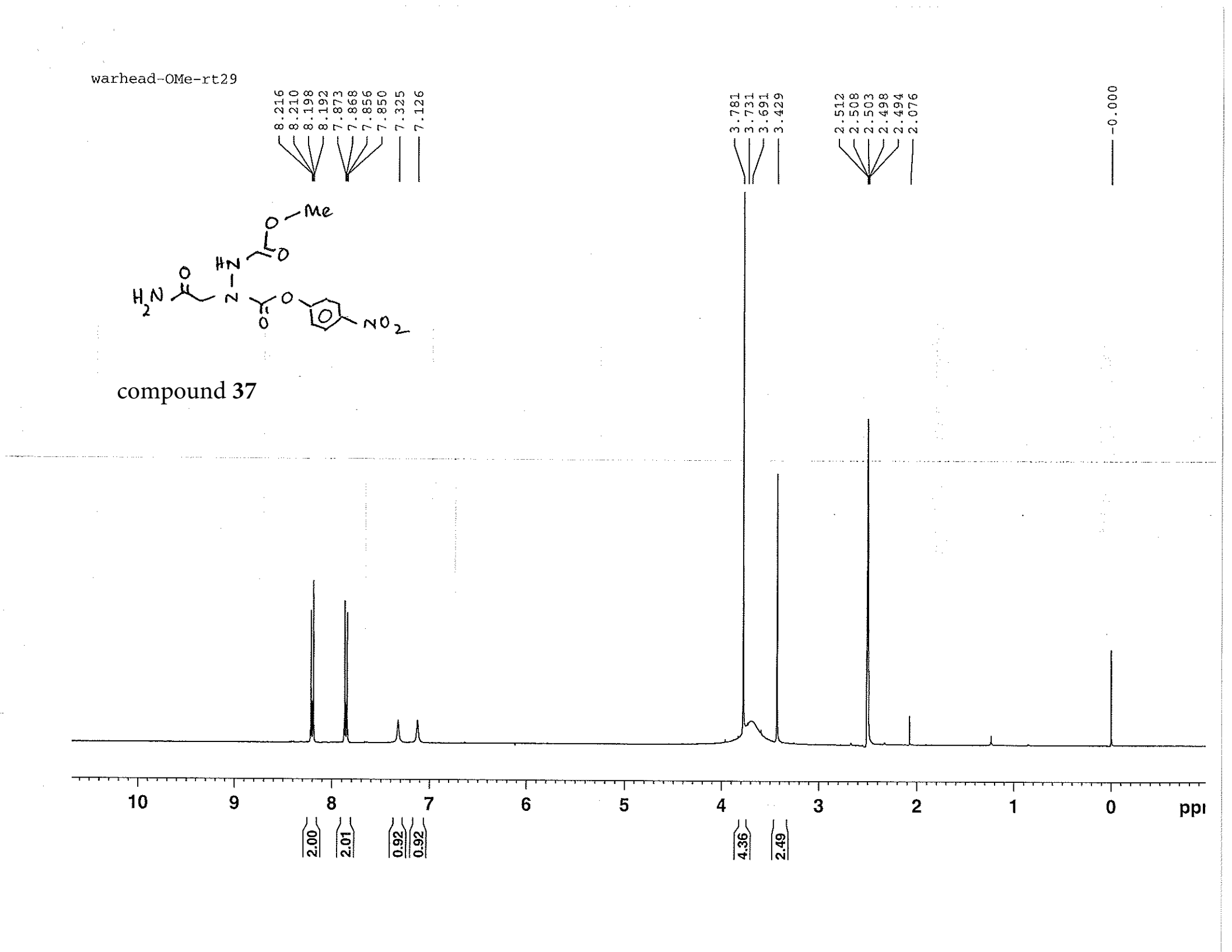
compound **35**

Br-Ph-thio-5-mem



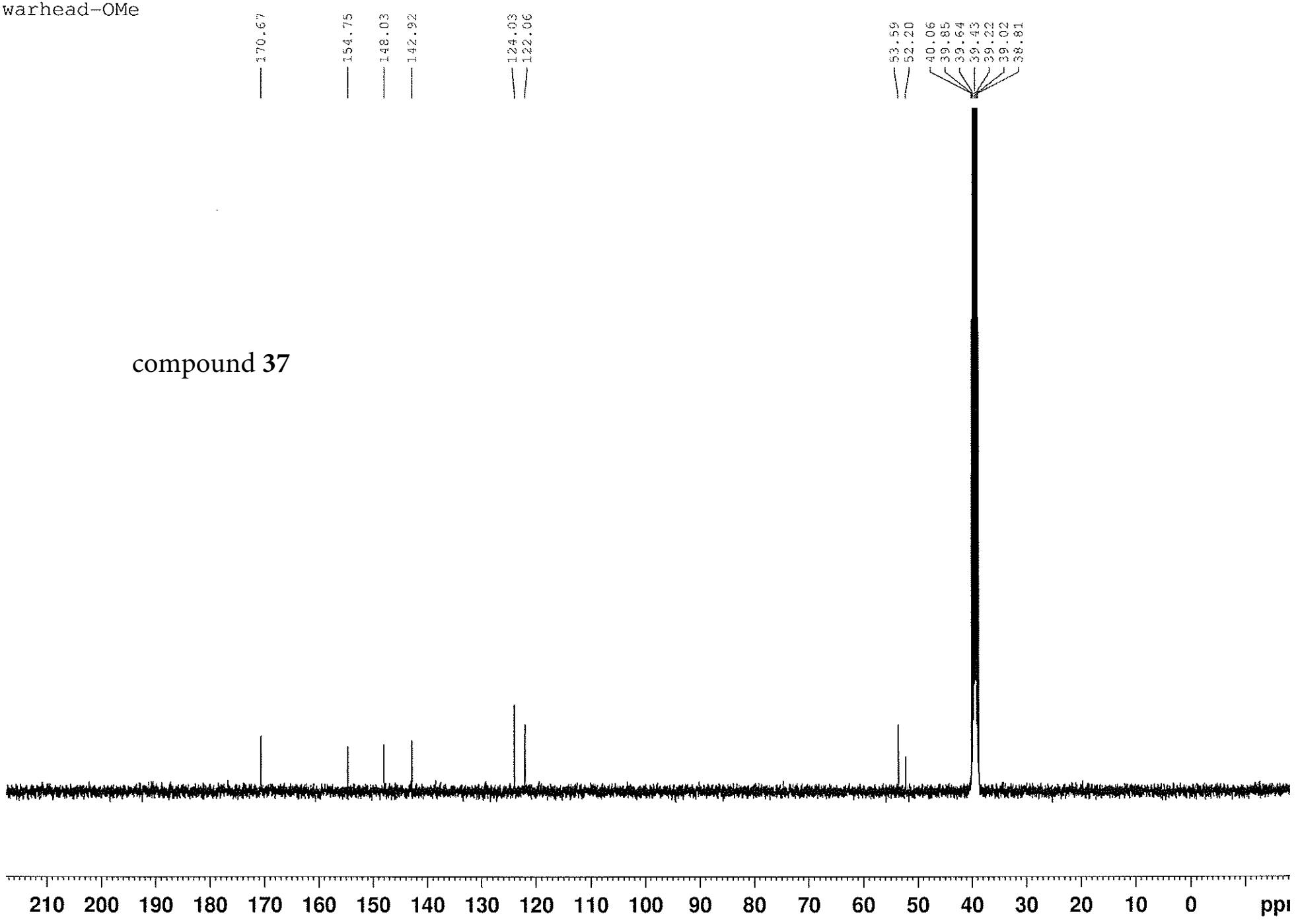
compound **35**

warhead-OMe-rt29



compound **37**

warhead-OMe



compound **37**