Supporting Information for the Manuscript

Highly Efficient Synthesis of Phenols by Copper-Catalyzed Oxidative Hydroxylation of Arylboronic Acids at Room Temperature in Water

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Page S03-S10 the experimental section.

Page S11-S50: the ^{1}H NMR and ^{13}C NMR spectra for compounds **2a-t.**

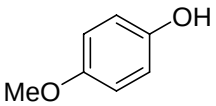
The ^{1}H NMR and ^{13}C NMR spectra were recorded on a JOEL JNM-ECA 300 spectrometer.

List of ^{1}H NMR and ^{13}C NMR spectra for compounds 2a-t.

Page S11	^{1}H NMR of **2a**	Page S12	^{13}C NMR of **2a**
Page S13	^{1}H NMR of **2b**	Page S14	^{13}C NMR of **2b**
Page S15	^{1}H NMR of **2c**	Page S16	^{13}C NMR of **2c**
Page S17	^{1}H NMR of **2d**	Page S18	^{13}C NMR of **2d**
Page S19	^{1}H NMR of **2e**	Page S20	^{13}C NMR of **2e**
Page S21	^{1}H NMR of **2f**	Page S22	^{13}C NMR of **2f**
Page S23	^{1}H NMR of **2g**	Page S24	^{13}C NMR of **2g**
Page S25	^{1}H NMR of **2h**	Page S26	^{13}C NMR of **2h**
Page S27	^{1}H NMR of **2i**	Page S28	^{13}C NMR of **2i**
Page S29	^{1}H NMR of **2j**	Page S30	^{13}C NMR of **2j**
Page S31	^{1}H NMR of **2k**	Page S32	^{13}C NMR of **2k**
Page S33	^{1}H NMR of **2l**	Page S34	^{13}C NMR of **2l**
Page S35	^{1}H NMR of **2m**	Page S36	^{13}C NMR of **2m**
Page S37	^{1}H NMR of **2n**	Page S38	^{13}C NMR of **2n**
Page S39	^{1}H NMR of **2o**	Page S40	^{13}C NMR of **2o**
Page S41	^{1}H NMR of **2p**	Page S42	^{13}C NMR of **2p**
Page S43	^{1}H NMR of **2q**	Page S44	^{13}C NMR of **2q**
Page S45	^{1}H NMR of **2r**	Page S46	^{13}C NMR of **2r**
Page S47	^{1}H NMR of **2s**	Page S48	^{13}C NMR of **2s**
Page S49	^{1}H NMR of **2t**	Page S50	^{13}C NMR of **2t**

Experimental Section

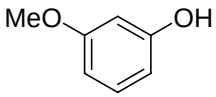
General Conditions: All melting points were determined on a Yanaco melting point apparatus and are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL JNM-ECA 300 spectrometer in $CDCl_3$ or CD_3OD. TMS was used as internal reference and the *J* values are given in Hz. PE is petroleum ether (60-90^{o}).



2a

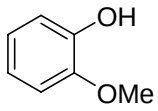
A Typical Procedure for Preparation of 4-Methoxyphenol (2a) by A Copper-Catalyzed Hydroxylation of 4-Methoxyphenylboronic Acid (1a): A mixture of $CuSO_4$ (16 mg, 0.1 mmol), 1,10-phenanthroline (36 mg, 0.2 mmol), 4-methoxypheny-boronic acid (**1a**, 152 mg. 1 mmol), KOH (168 mg, 3.0 mmol) in H_2O (5 mL) was stirred for 2 h at room temperature in open to air (without bubbling air). After **1a** was exhausted completely (monitored by TLC), the reaction was cooled to 0 ^{o}C and quenched carefully by aqueous solution of HCl (2 M, 15 mL). The resultant mixture was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine (20 mL) and dried over Na_2SO_4. After removal of the solvent in vacuun, the residue was purified by chromatography (silica gel, EtOAc:PE = 1:5) to give desired product **2a** (117 mg, 94%) as a colorless solid, mp 57-58 ^{o}C (EtOAc-PE) (lit.[6] 58 ^{o}C). ^{1}H NMR ($CDCl_3$): δ6.78 (d, *J* = 1.7, 4H), 4.78 (s, 1H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$): δ153.4, 149.4, 116.1 (2C), 114.9 (2C), 55.9.

By the similar procedure, products **2b-t** were prepared (see Scheme 2 in the text).



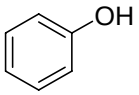
2b

3-Methoxyphenol (2b).[4] It was a colorless oil, ^{1}H NMR ($CDCl_3$): δ7.10 (t, J = 7.9, 1H), 6.50-6.41 (m, 3H), 6.32 (s, 1H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$): δ160.6, 156.6, 130.2, 108.0, 106.4, 101.5, 55.2.



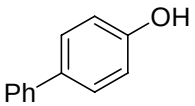
2c

2-Methoxyphenol (2c). It was a white solid, mp 28-29 ^{o}C (EtOAc-PE) (lit.[3] 27-28 ^{o}C). ^{1}H NMR ($CDCl_3$): δ6.94-6.91 (m, 1H), 6.86-6.82 (m, 3H), 5.75 (s, 1H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$): δ146.5, 145.5, 121.3, 120.1, 114.5, 110.7, 55.7.



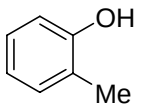
2d

Phenol (2d). it was a colorless solid, mp 41-42 ^{o}C (EtOAc-PE) (lit.[1] 41-42 ^{o}C). ^{1}H NMR ($CDCl_3$): δ7.28-7.22 (m, 2H), 6.96-6.91 (m, 1H), 6.85-6.82 (m, 2H), 5.03 (s, 1H); ^{13}C NMR ($CDCl_3$): δ155.0, 129.7 (2C), 121.0, 115.3 (2C).



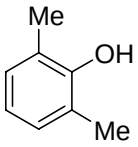
2e

4-Phenylphenol (2e). It was a yellowish solid, mp 165-167 ^{o}C (EtOAc-PE) (lit.[6] 165 ^{o}C). ^{1}H NMR (CD_3OD): δ 7.48 (d, J = 5.4, 2H), 7.40 (dd, J = 8.6, 2.1, 2H), 7.32 (dt, J = 6.3, 1.6, 2H), 7.22-7.18 (m, 1H), 6.83 (dd, J = 6.5, 2.1, 2H); ^{13}C NMR (CD_3OD): δ 158.1, 142.4, 133.8, 129.7 (2C), 129.0 (2C), 127.4 (3C), 116.6 (2C).



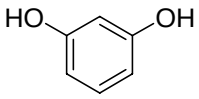
2f

2-MethylPhenol (2f). It was a white solid, mp 31-32 ^{o}C (EtOAc-PE) (lit.[2] 30-32 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.13-7.05 (m, 2H), 6.84 (t, J = 7.4, 1H), 6.76 (d, J = 7.9, 1H), 4.89 (s, 1H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$): δ 153.7, 131.0, 127.1, 123.7, 120.7, 114.9, 15.7.



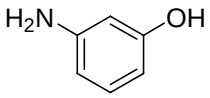
2g

2,6-Dimethylphenol (1g). It was a white solid, mp 42-43 ^{o}C (EtOAc-PE) (lit.[4] 44-45 ^{o}C). ^{1}H NMR (CD_3OD): δ 6.97 (d, J = 7.2, 2H), 6.75 (t, J = 7.6, 1H), 4.62 (s, 1H), 2.23 (s, 6H); ^{13}C NMR (CD_3OD): δ 152.1, 128.6 (2C), 122.9, 120.2 (2C), 15.8 (2C).



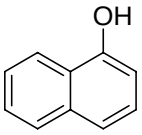
2h

Benzene-1,3-diol (2h). It was a white solid, mp 111-112 ^{o}C (EtOAc-PE) (lit.[7] 107-109 ^{o}C). ^{1}H NMR (CD_3OD): δ 6.96-6.90 (m, 1H), 6.27-6.24 (m, 3H); ^{13}C NMR (CD_3OD): δ 159.4 (2C), 130.9, 107.7 (2C), 103.4.



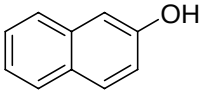
2i

3-Aminophenol (2i). It was a grey white solid, mp 117-118 ^{o}C (EtOAc-PE) (lit.[5] 119-120 ^{o}C); ^{1}H NMR (CD_3OD): δ 6.91-6.85 (m, 1H), 6.23-6.14 (m, 3H); ^{13}C NMR (CD_3OD): δ 159.1, 149.8, 130.8, 108.6, 106.6, 103.7.



2j

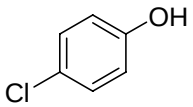
1-Naphthalenol (2j). It was a yellowish solid, mp 91-93 ^{o}C (EtOAc-PE) (lit.[14] 92-94 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 8.18-8.13 (m, 1H), 7.82-7.77 (m, 1H), 7.50-7.41 (m, 3H), 7.30 (t, J = 7.5, 1H), 6.81 (d, J = 7.2, 1H), 5.27 (s, 1H); ^{13}C NMR ($CDCl_3$): δ 151.2, 134.7, 127.7, 126.4, 125.8, 125.3, 124.3, 121.5, 120.7, 108.7.



2k

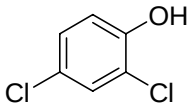
2-Naphthalenol (2k). It was a white solid, mp 122-124 ^{o}C (EtOAc-PE) (lit.[6] 122^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.76-7.71 (m, 2H), 7.65 (d, J = 8.3, 1H), 7.41 (d, J = 7.2,

1H), 7.33-7.29 (m, 1H), 7.11-7.05 (m, 2H), 5.32 (s, 1H); ^{13}C NMR ($CDCl_3$): δ153.2, 134.5, 129.8, 128.9, 127.7, 126.5, 126.3, 123.6, 117.7, 109.5.



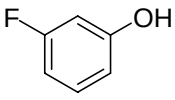
2l

4-Chlorophenol (2l). It was a white solid, mp 44-45 ^{o}C (EtOAc-PE) (lit.[12] 43 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.23 (d, J = 8.6, 2H), 6.77 (d, J = 8.6, 2H), 4.86 (s, 1H); ^{13}C NMR ($CDCl_3$): δ153.6, 129.5 (2C), 125.8, 116.6 (2C).



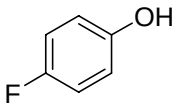
2m

2,4-Dichlorophenol (2m). It was a white solid, mp 43-44 ^{o}C (EtOAc-PE) (lit.[13] 41-44 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.31 (d, J = 2.4, 1H), 7.14 (dd, J = 8.8, 2.7, 1H), 6.95 (d, J = 9.0, 1H), 5.56 (s, 1H); ^{13}C NMR ($CDCl_3$): δ150.1, 128.5, 128.4, 125.5, 120.4, 117.1.



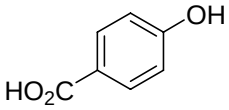
2n

3-Fluorophenol (2n).[9] It was a colorless oil. ^{1}H NMR ($CDCl_3$): δ7.19-7.12 (m, 1H), 6.66-6.59 (m, 2H), 6.57-6.55 (m, 1H), 6.37 (br, 1H); ^{13}C NMR ($CDCl_3$): δ163.6 (d, J = 243.8), 156.7 (d, J = 11.5), 130.5 (d, J = 10.1), 111.2 (d, J = 2.9), 107.7 (d, J = 21.5), 103.2 (d, J = 24.4).



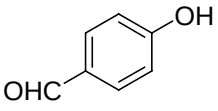
2o

4-Fluorophenol (2o). It was a white solid, mp 46-47 ^{o}C (EtOAc-PE) (lit.[11] 46 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 6.95-6.88 (m, 2H), 6.80-6.75 (m, 2H), 5.91 (br, 1H); ^{13}C NMR ($CDCl_3$): δ 157.2 (d, J = 235.9), 151.4, 116.2 (d, J = 10.0, 2C), 116.0 (d, J = 22.9, 2C).



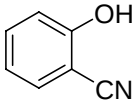
2p

4-Hydroxybenzoic acid (2p). It was a white solid, mp 215-217 ^{o}C (MeOH-CH_2Cl_2) (lit.[15] 213-214 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.78-7.73 (m, 2H), 6.72-6.67 (m, 2H); ^{13}C NMR ($CDCl_3$): δ 170.1, 163.3, 133.0 (2C), 122.6, 116.0 (2C).



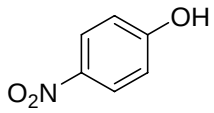
2q

4-Hydroxybenzaldehyde (2q). It was a yellowish solid, mp 114-116 ^{o}C (EtOAc-PE) (lit.[4] 113-117 ^{o}C). ^{1}H NMR (CD_3OD): δ 9.69 (s, 1H), 7.70 (d, J = 8.6, 2H), 6.85 (d, J = 8.4, 2H); ^{13}C NMR (CD_3OD): δ 192.8, 165.1, 133.4 (2C), 130.3, 116.8 (2C).



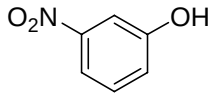
2r

2-Hydroxybenzonitrile (2r). It was a grey white solid, mp 96-98 ^{o}C (EtOAc-PE) (lit.[8] 99-100 ^{o}C). ^{1}H NMR (CD_3OD): δ 7.49-7.40 (m, 2H), 6.95-6.88 (m, 2H); ^{13}C NMR (CD_3OD): δ 161.5, 135.6, 134.3, 120.8, 117.8, 117.0, 100.6.



2s

4-Nitrophenol (2s). It was a yellowish solid, mp 113-114 ^{o}C (EtOAc-PE) (lit.[14] 110 ^{o}C). ^{1}H NMR (CD_3OD): δ 7.99-7.95 (m, 2H), 6.76-6.72 (m, 2H); ^{13}C NMR (CD_3OD): δ 165.1, 141.7, 127.0 (2C), 116.4 (2C).



2t

3-Nitrophenol (2t). It was a yellowish solid, mp 98-99 ^{o}C (EtOAc-PE) (lit.[10] 95 ^{o}C). ^{1}H NMR ($CDCl_3$): δ 7.82-7.79 (m, 1H), 7.73 (t, J = 2.4, 1H), 7.41 (t, J = 8.2, 1H), 7.23-7.20 (m, 1H), 6.15 (br, 1H); ^{13}C NMR ($CDCl_3$): δ 156.3, 149.0, 130.3, 122.1, 115.8, 110.5.

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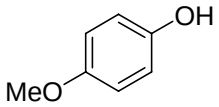
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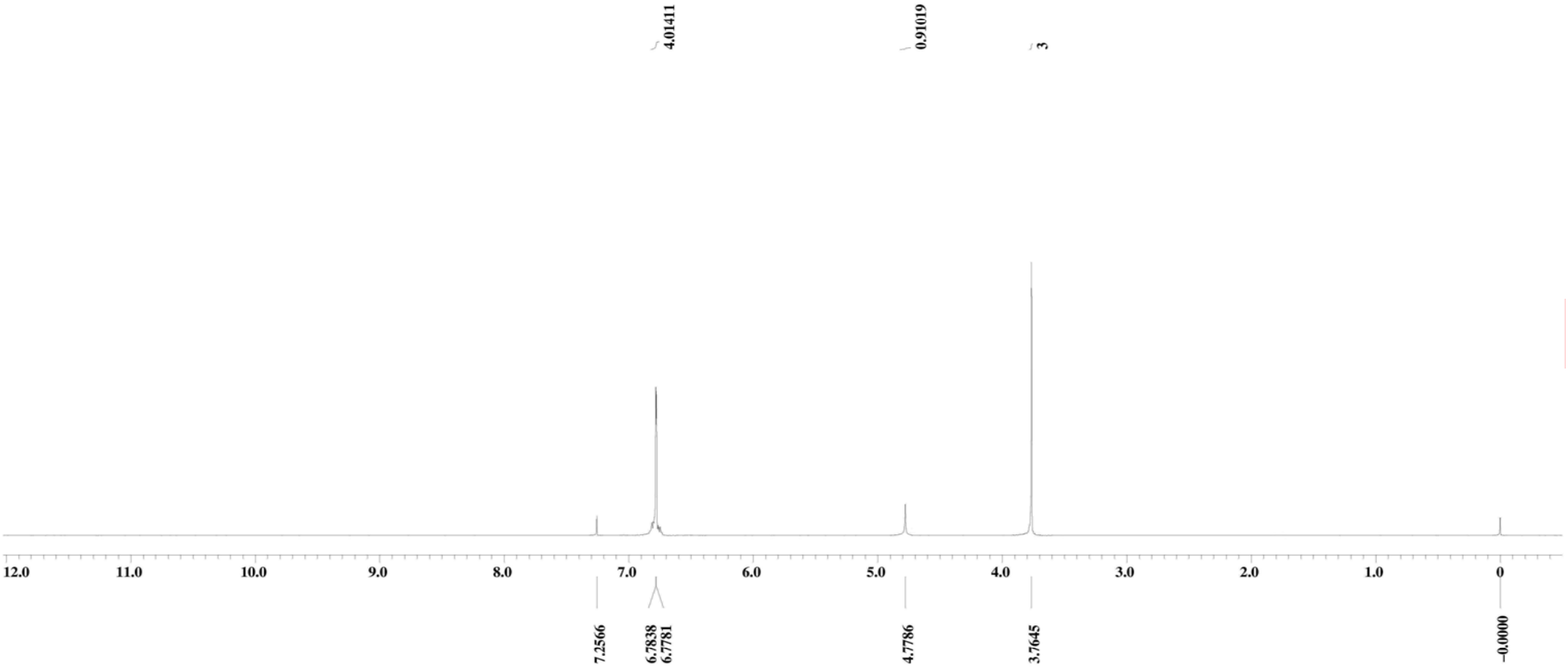
2a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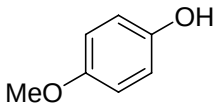
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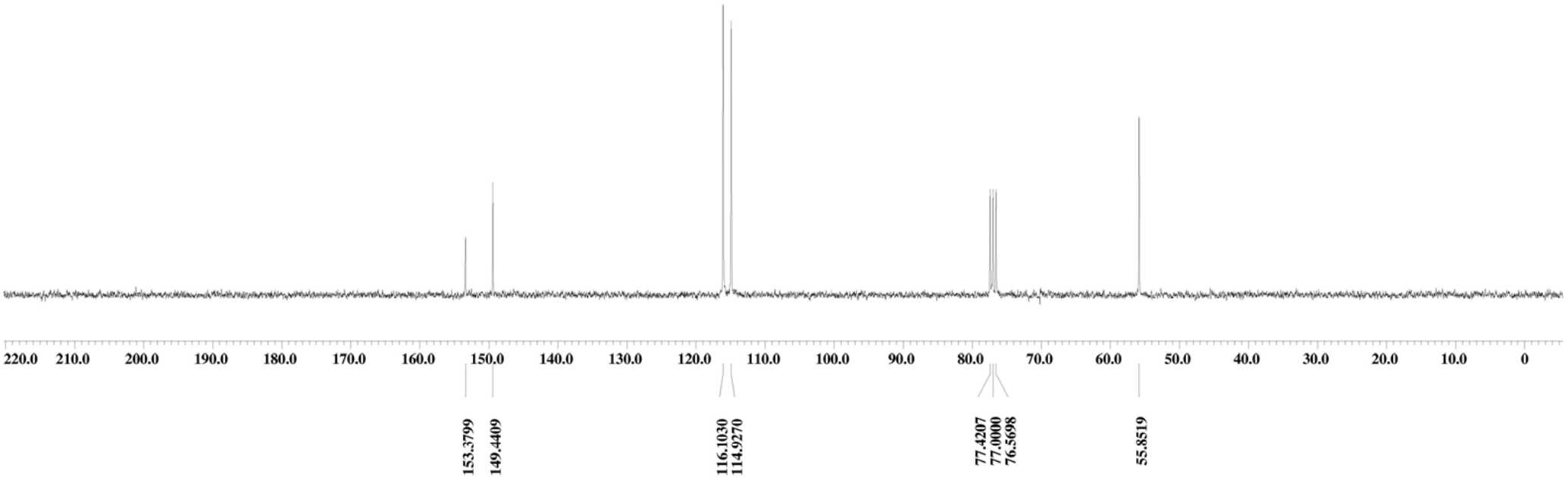
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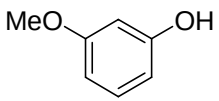
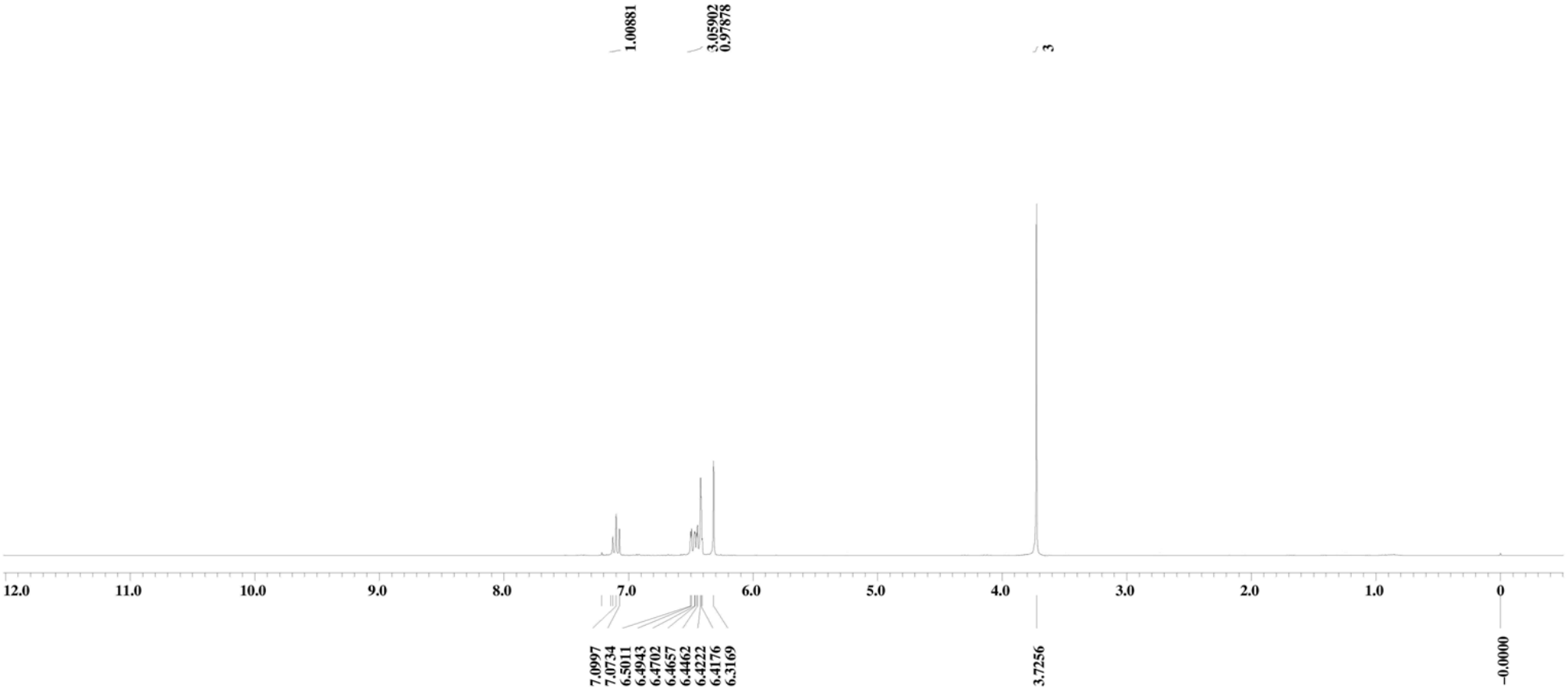

MeO
OH

2b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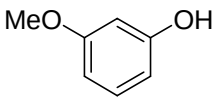
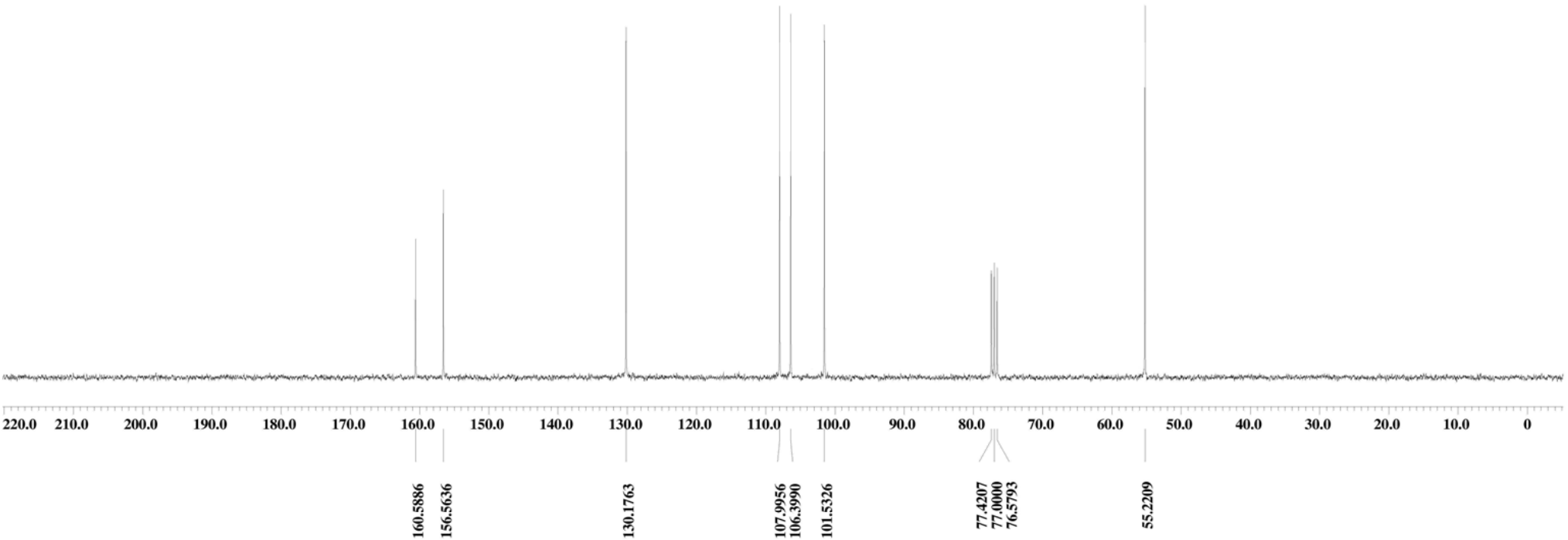
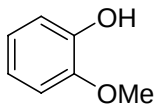
3.05902
0.97878
3
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.0997
7.0734
6.5011
6.4943
6.4702
6.4657
6.4462
6.4222
6.4176
6.3169
3.7256
-0.0000
X : parts per Million : 1H

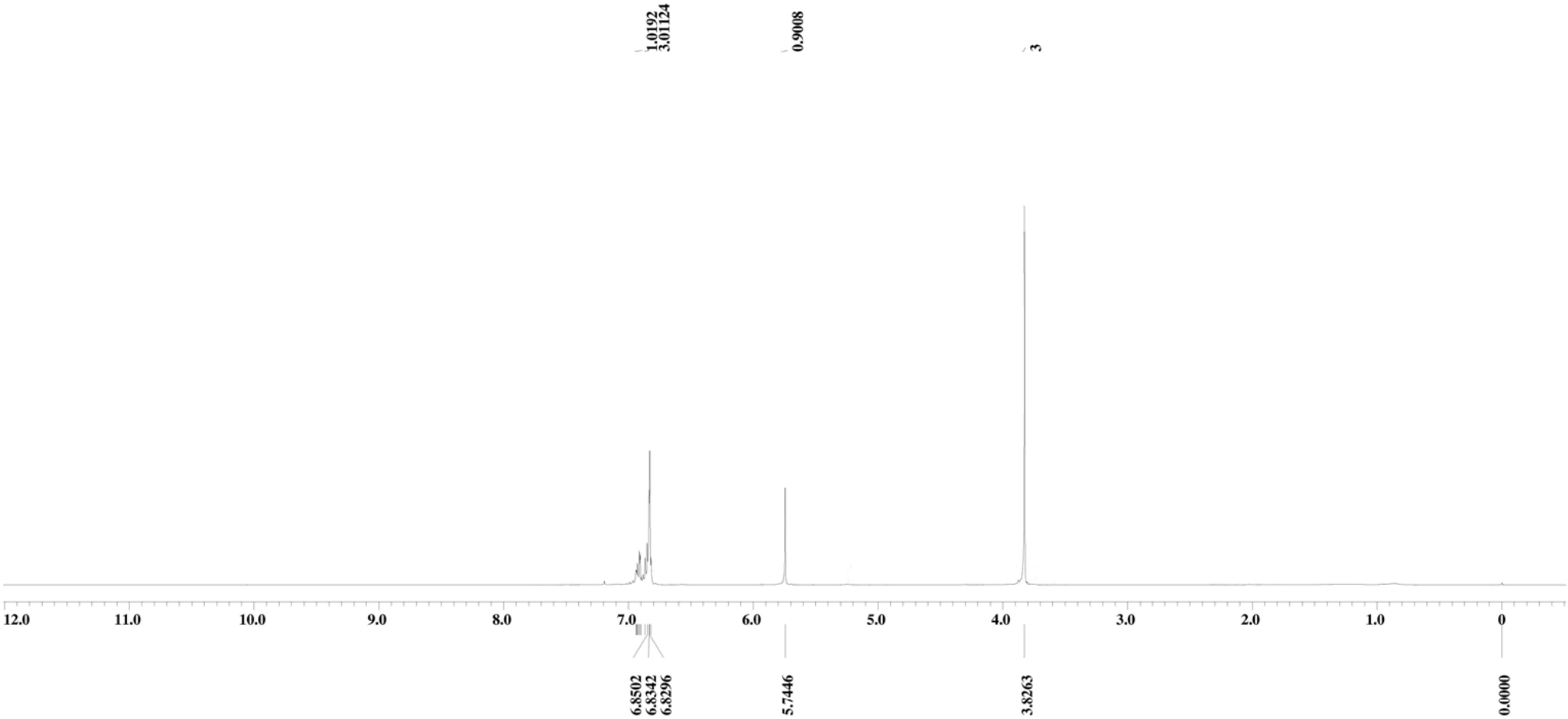

MeO
OH

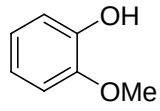
2b


220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
160.5886
156.5636
130.1763
107.9956
106.3990
101.5326
77.4207
77.0000
76.5793
55.2209
X : parts per Million : 13C

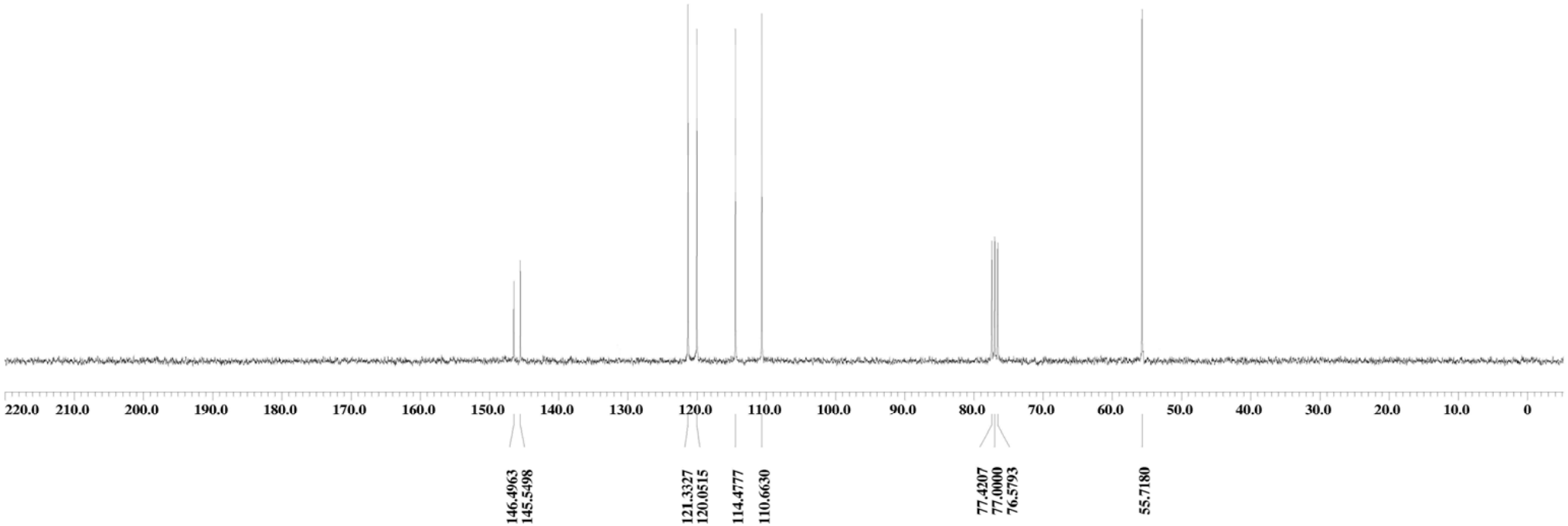

OH
OMe

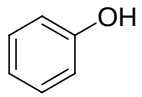
2c


1.0192
3.01124
0.9008
3
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.8502
6.8342
6.8296
5.7446
3.8263
0.0000
X : parts per Million : 1H

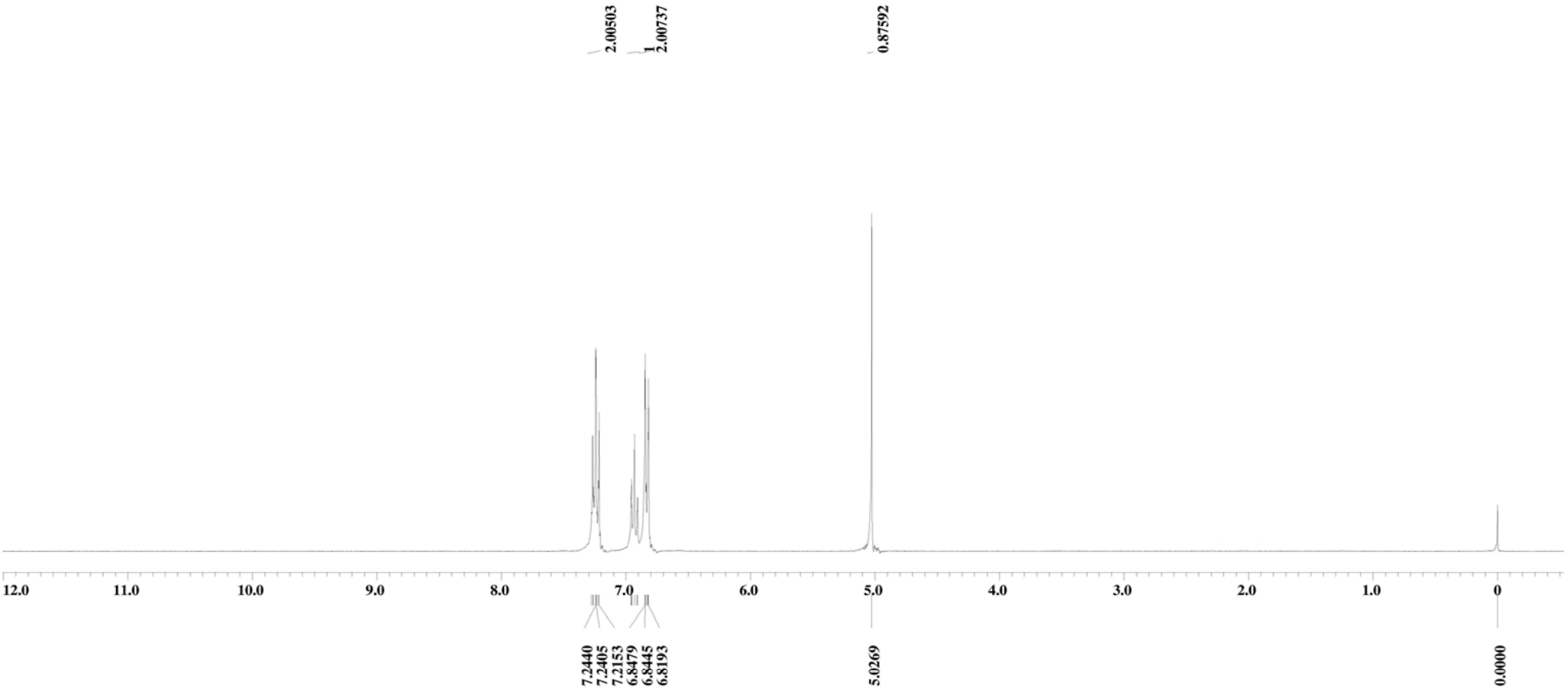

OH
OMe

2c

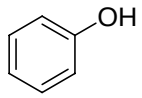

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
146.4963
145.5498
121.3327
120.0515
114.4777
110.6630
77.4207
77.0000
76.5793
55.7180
X : parts per Million : 13C



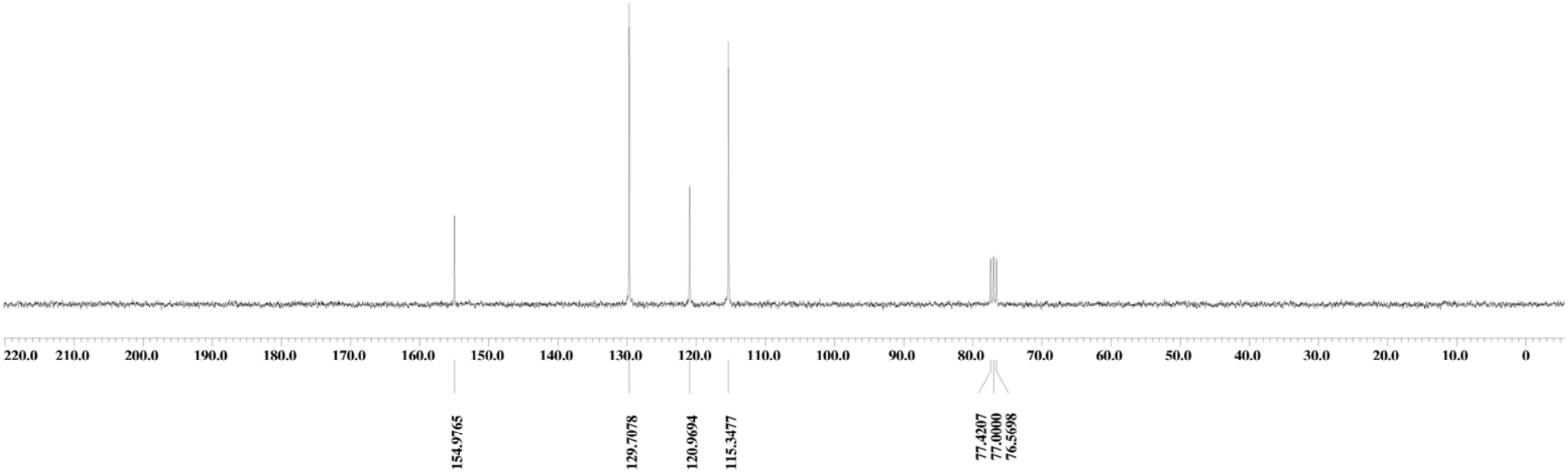
2d



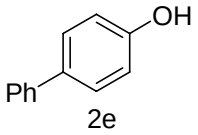
X : parts per Million : 1H



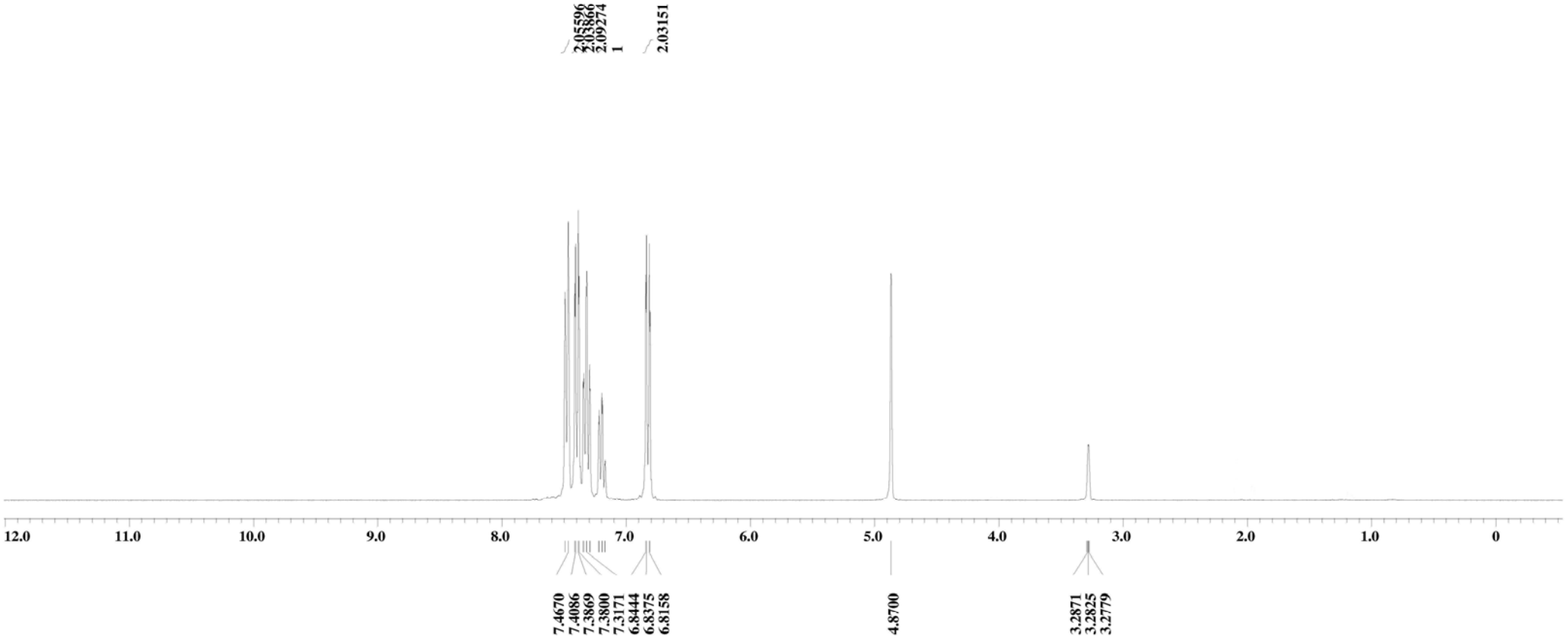
2d



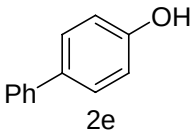
X : parts per Million : 13C



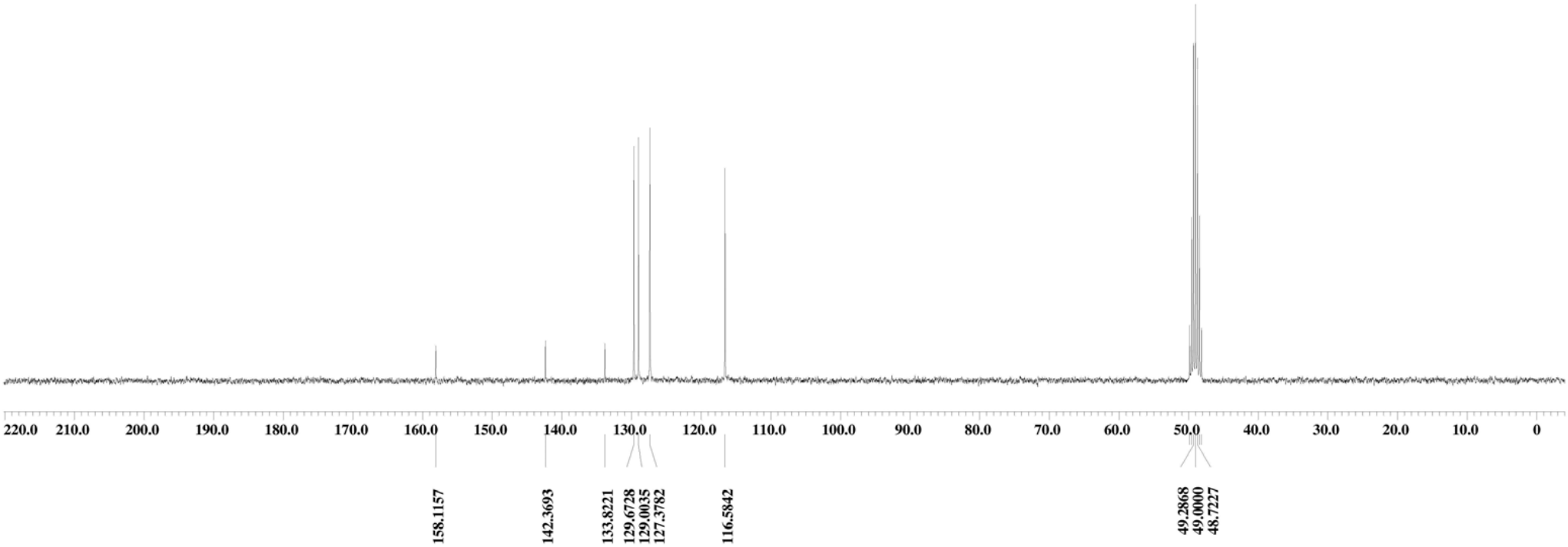
2e



X : parts per Million : 1H


OH
Ph

2e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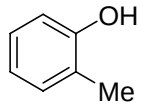
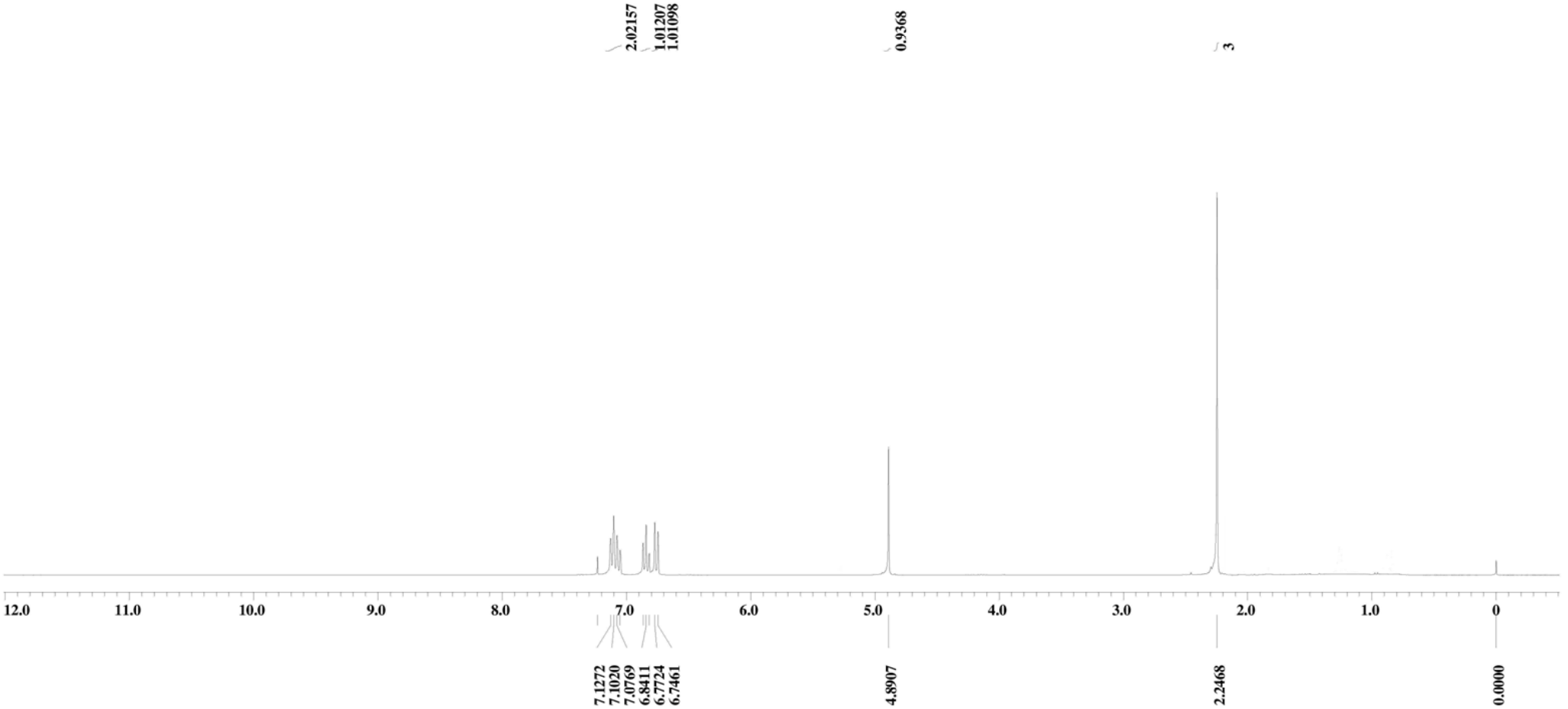
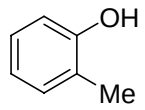
158.1157
142.3693
133.8221
129.6728
129.0035
127.3782
116.5842
49.2868
49.0000
48.7227
X : parts per Million : 13C

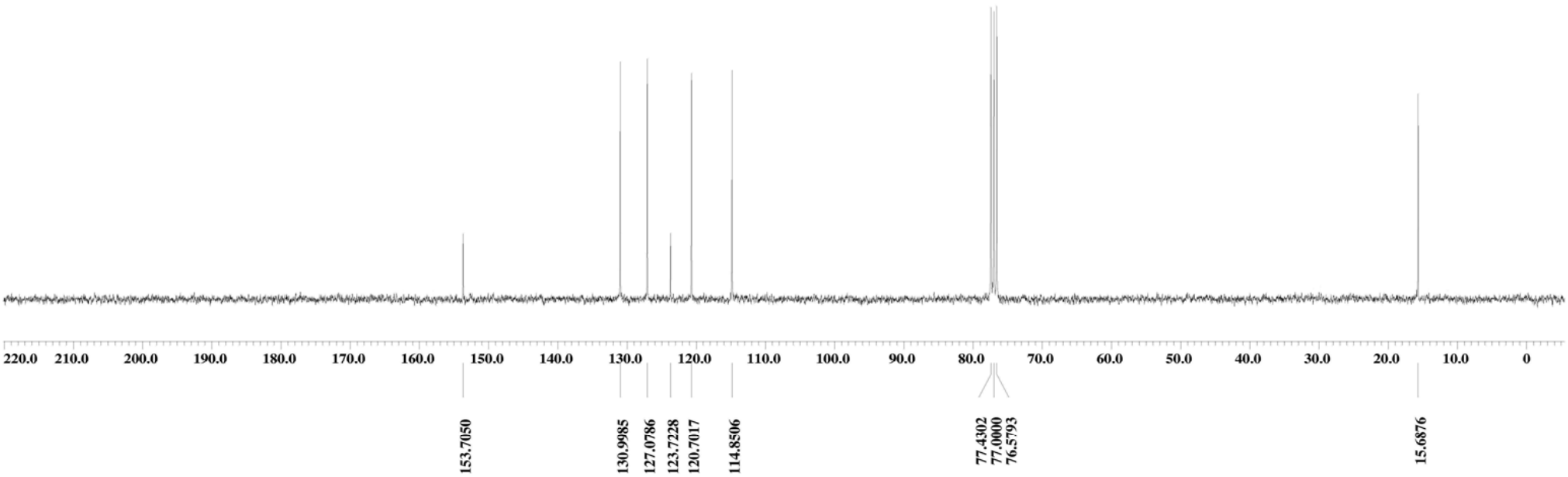

OH
Me

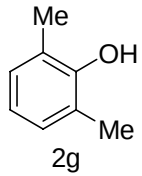
2f


2.02157
1.01207
1.01098
0.9368
3
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.1272
7.1020
7.0769
6.8411
6.7724
6.7461
4.8907
2.2468
0.0000
X : parts per Million : 1H

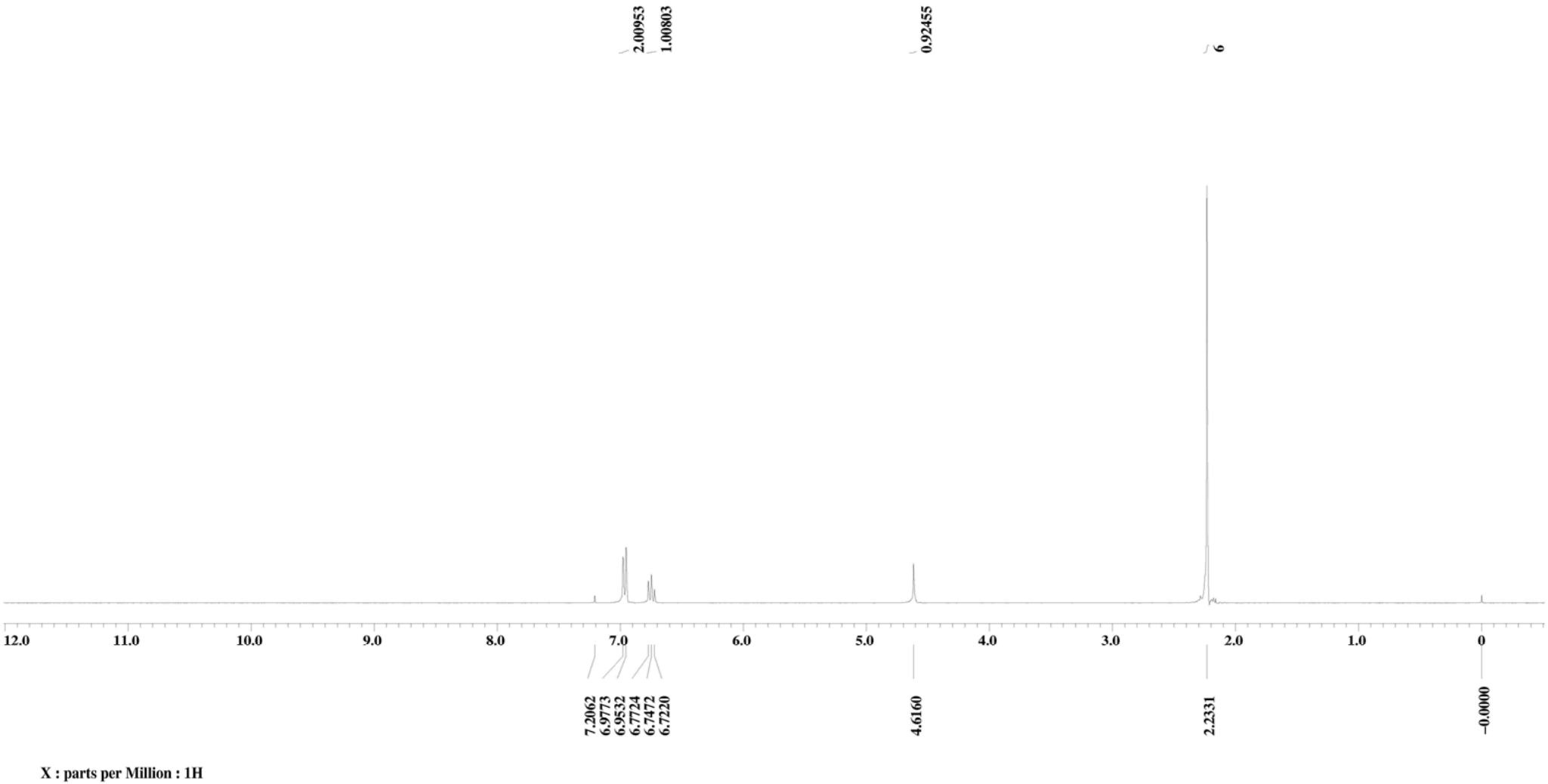

OH
Me

2f


220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
153.7050
130.9985
127.0786
123.7228
120.7017
114.8506
77.4302
77.0000
76.5793
15.6876
X : parts per Million : 13C


Me
OH
Me

2g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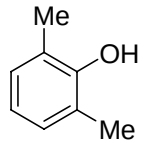
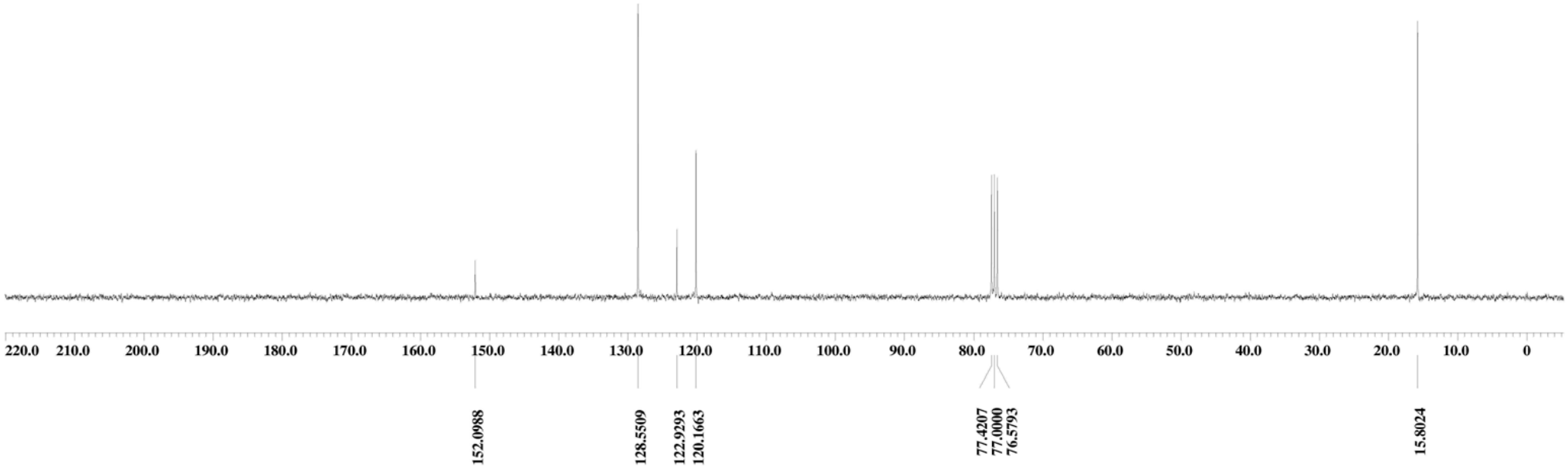
1.00803
0.92455
6
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2062
6.9773
6.9532
6.7724
6.7472
6.7220
4.6160
2.2331
-0.0000
X : parts per Million : 1H


Me
OH
Me

2g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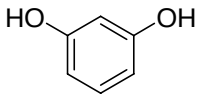
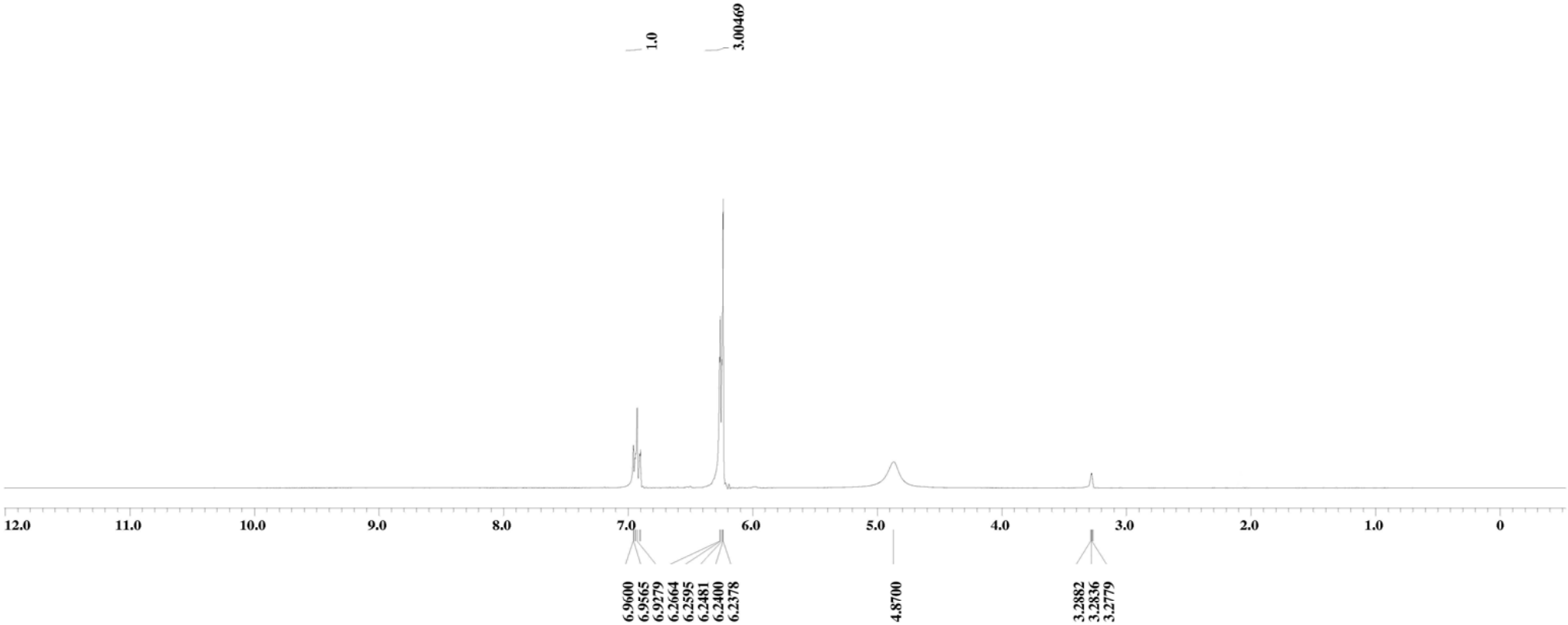
152.0988
128.5509
122.9293
120.1663
77.4207
77.0000
76.5793
15.8024
X : parts per Million : 13C


HO
OH

2h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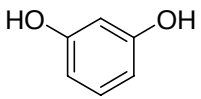
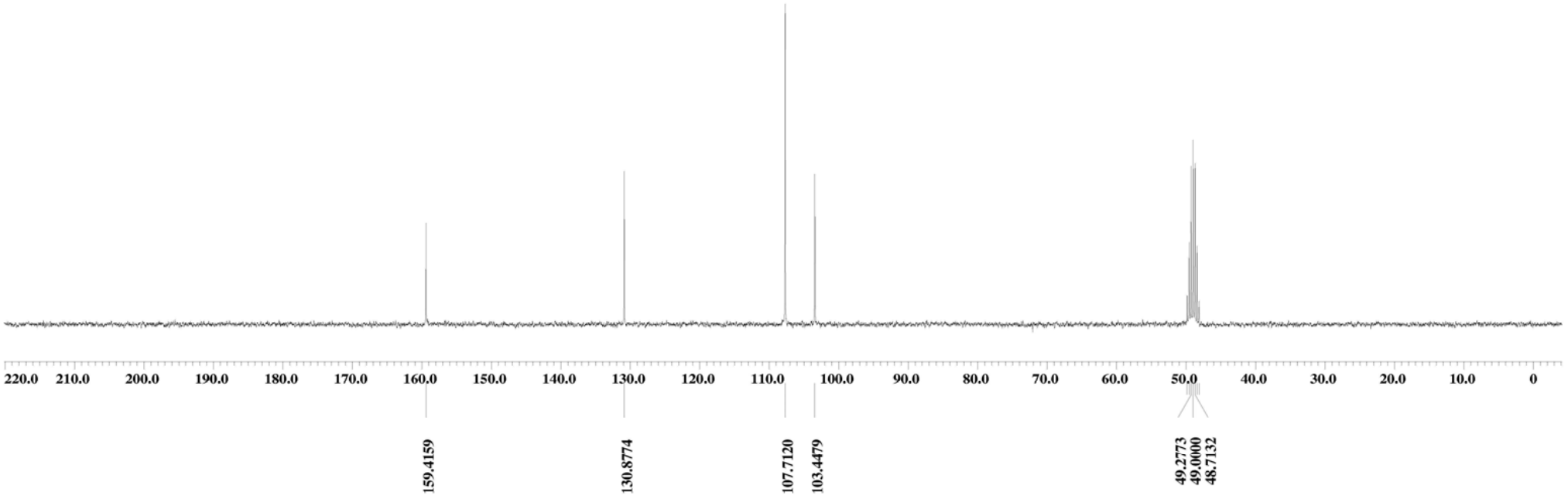
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.9600
6.9565
6.9279
6.2664
6.2595
6.2481
6.2400
6.2378
4.8700
3.2882
3.2836
3.2779
X : parts per Million : 1H


HO
OH

2h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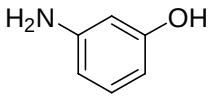
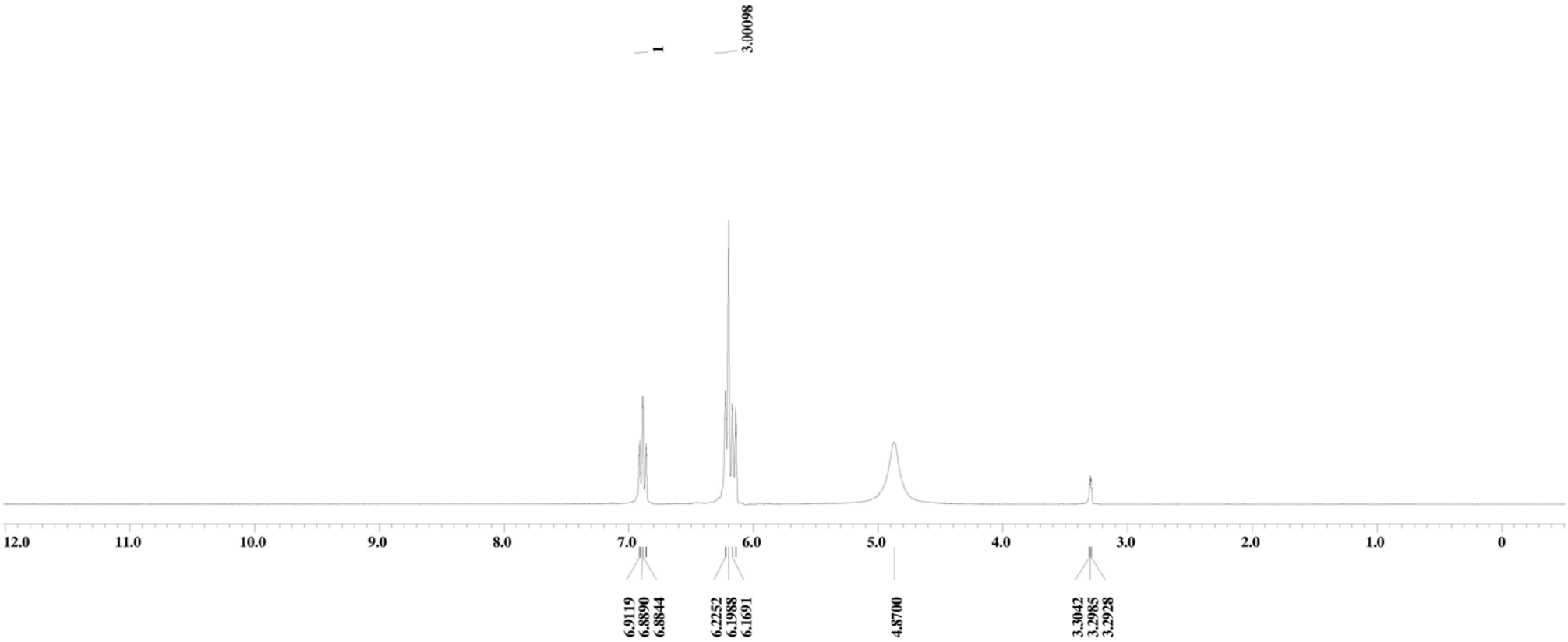
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.4159
130.8774
107.7120
103.4479
49.2773
49.0000
48.7132
X : parts per Million : 13C


H2N
OH

2i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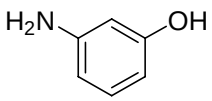
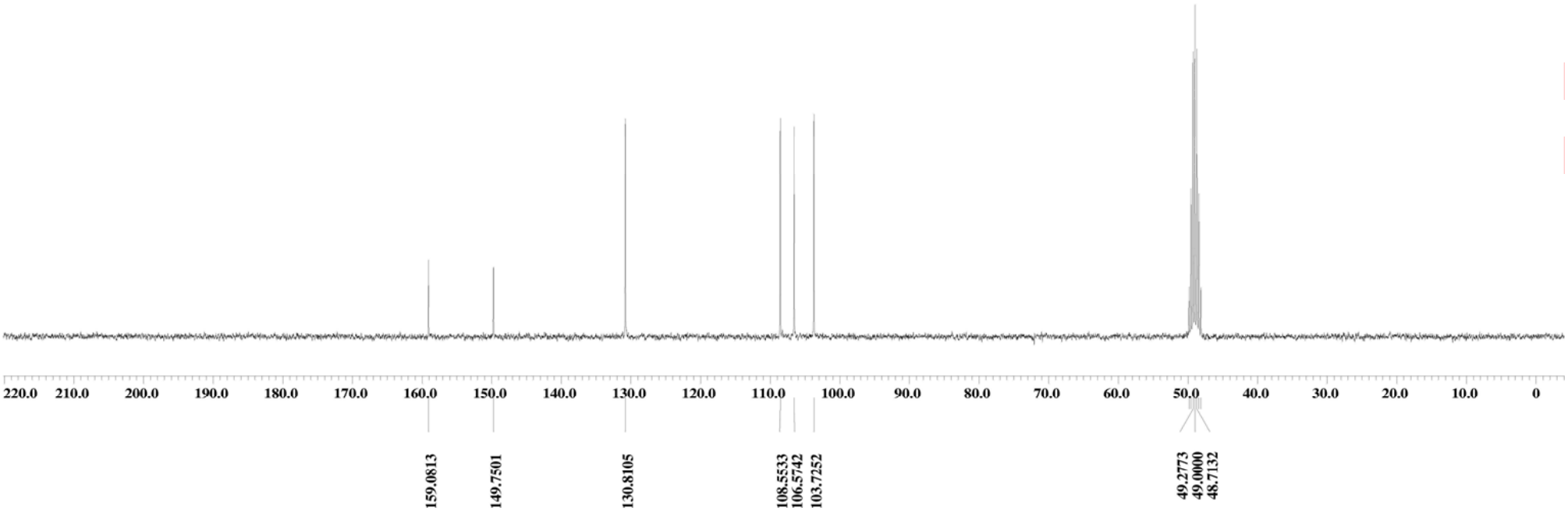
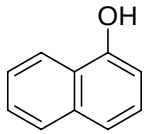
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.9119
6.8890
6.8844
6.2252
6.1988
6.1691
4.8700
3.3042
3.2985
3.2928
X : parts per Million : 1H

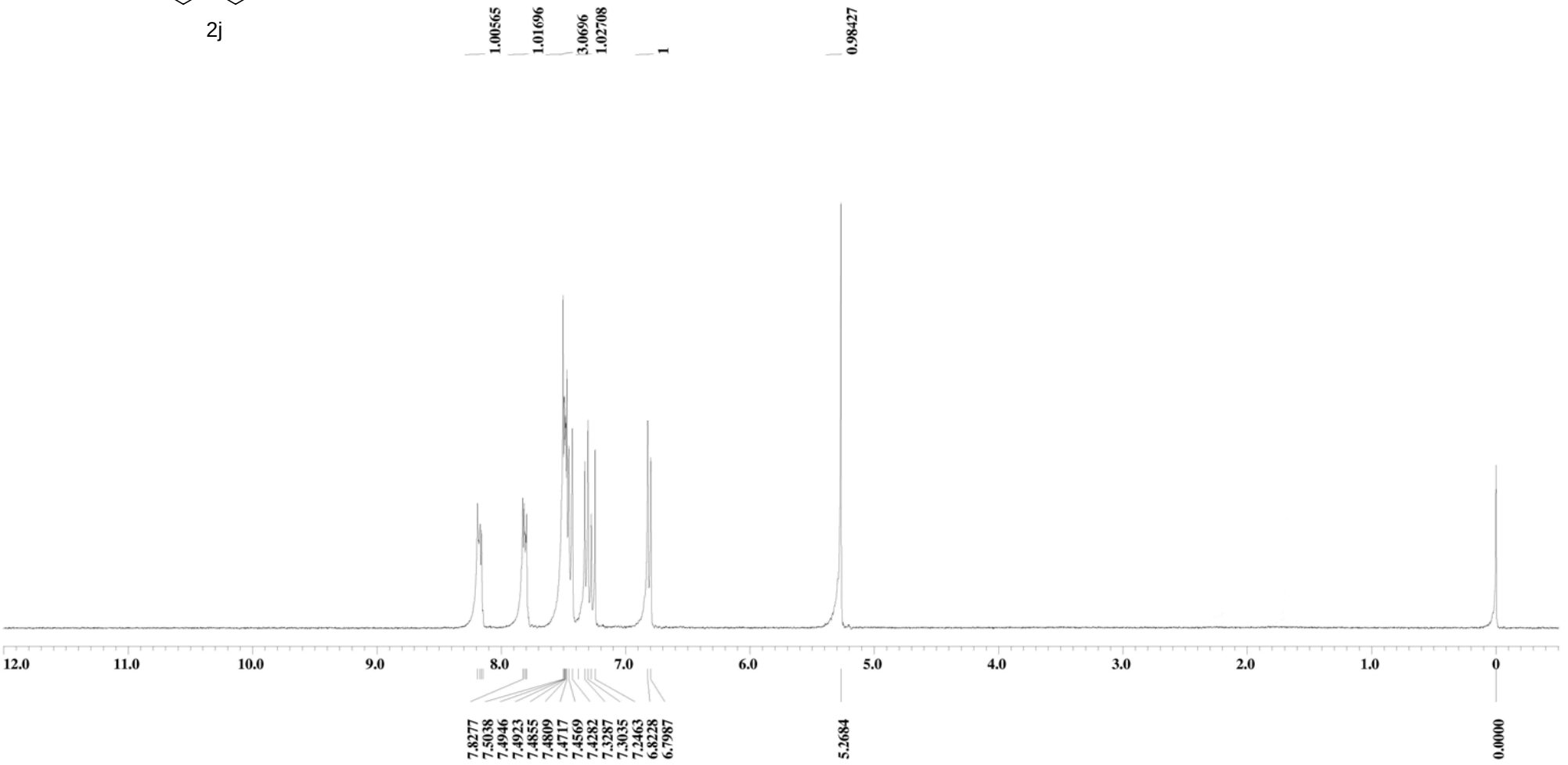

H2N
OH

2i


220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
159.0813
149.7501
130.8105
108.5533
106.5742
103.7252
49.2773
49.0000
48.7132
X : parts per Million : 13C


OH

2j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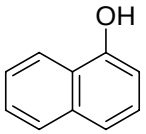
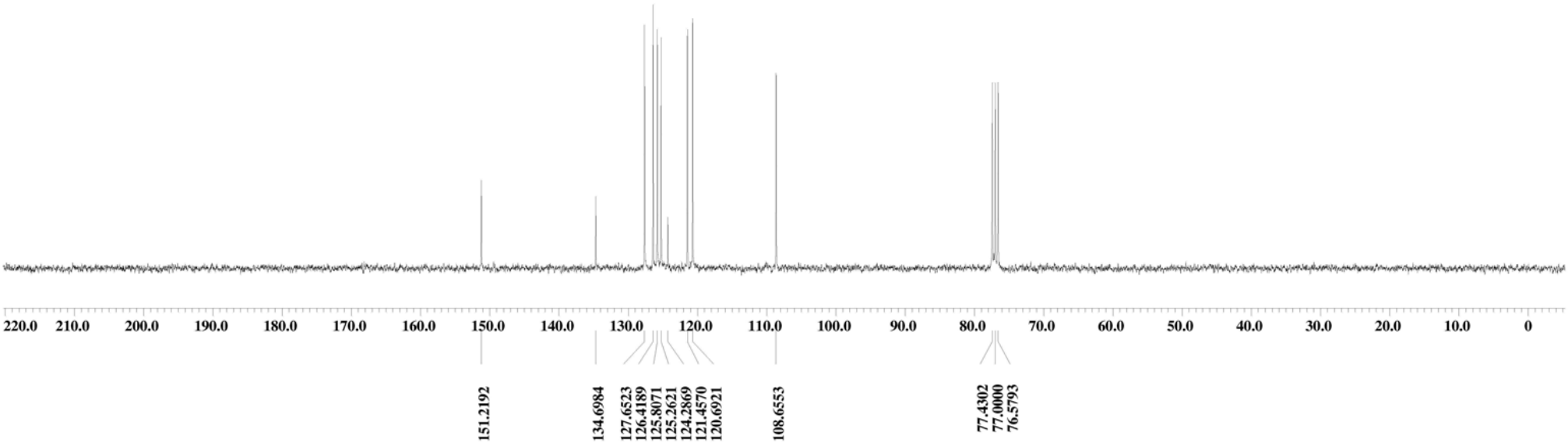
1.01696
3.0696
1.02708
1
0.98427
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8277
7.5038
7.4946
7.4923
7.4855
7.4809
7.4717
7.4569
7.4282
7.3287
7.3035
7.2463
6.8228
6.7987
5.2684
0.0000
X : parts per Million : 1H


OH

2j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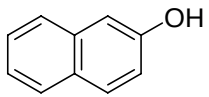
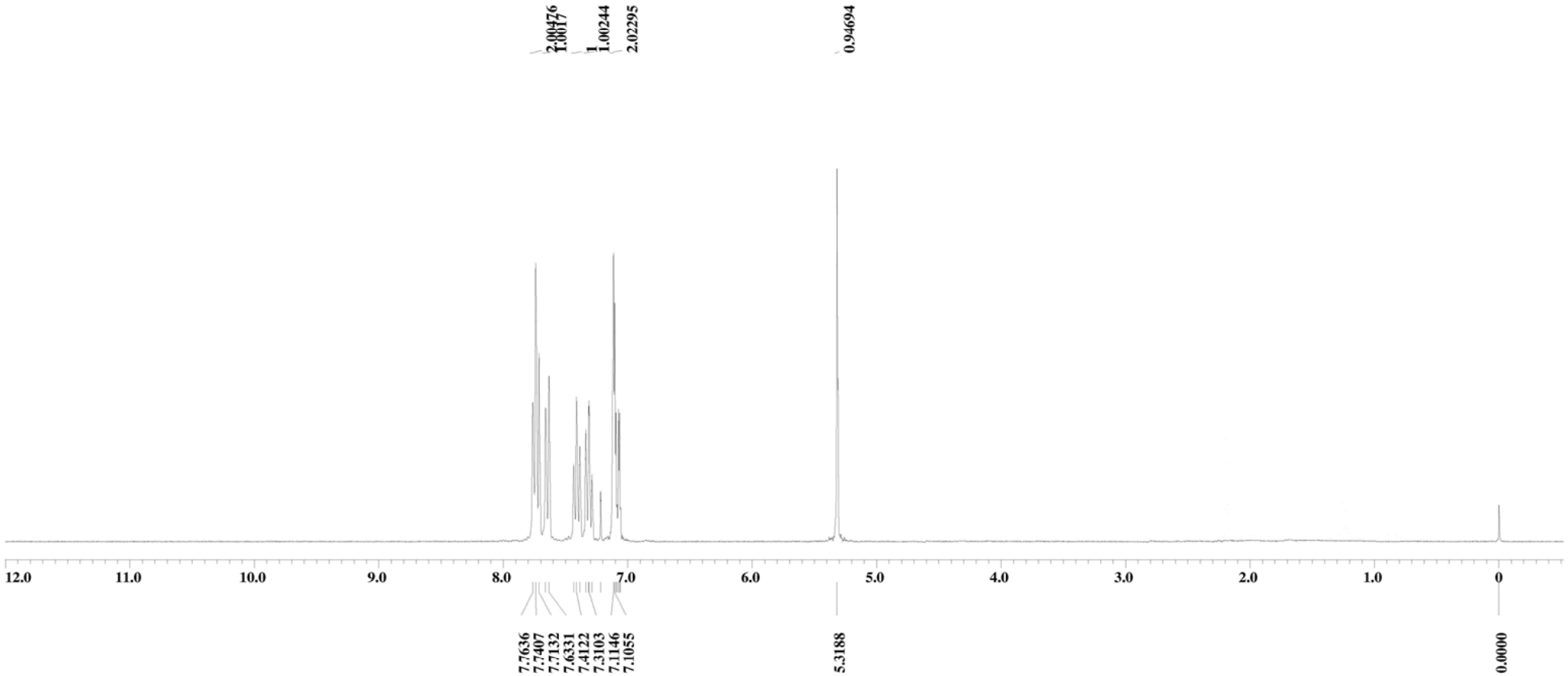
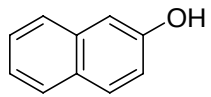
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
151.2192
134.6984
127.6523
126.4189
125.8071
125.2621
124.2869
121.4570
120.6921
108.6553
77.4302
77.0000
76.5793
X : parts per Million : 13C



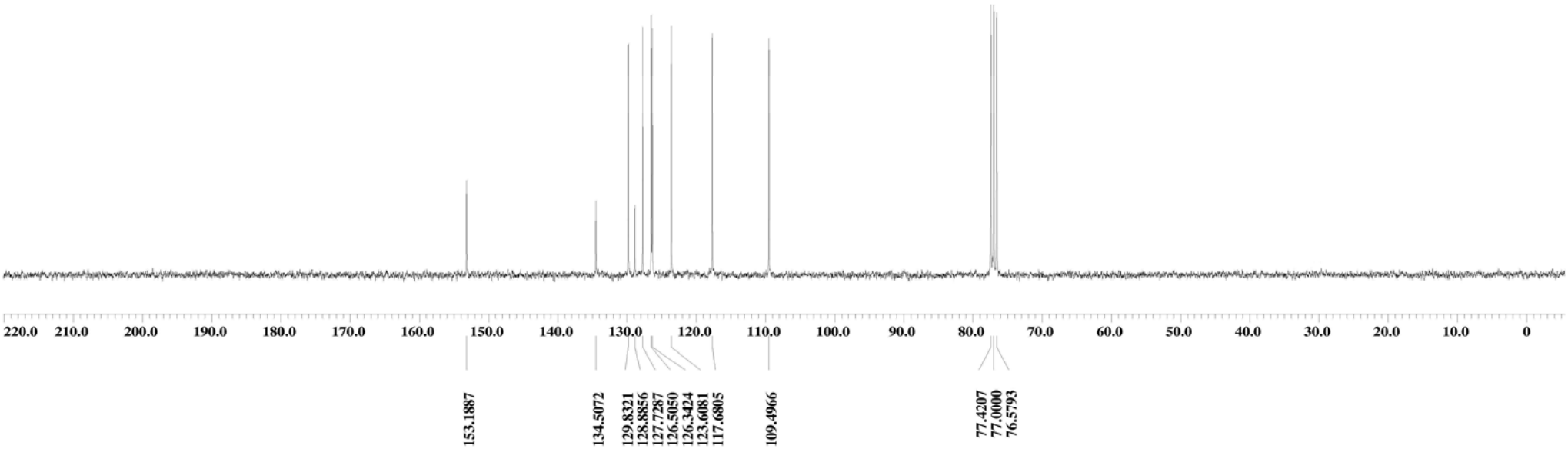
2k

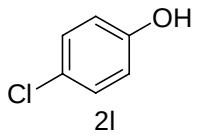


X : parts per Million : 1H

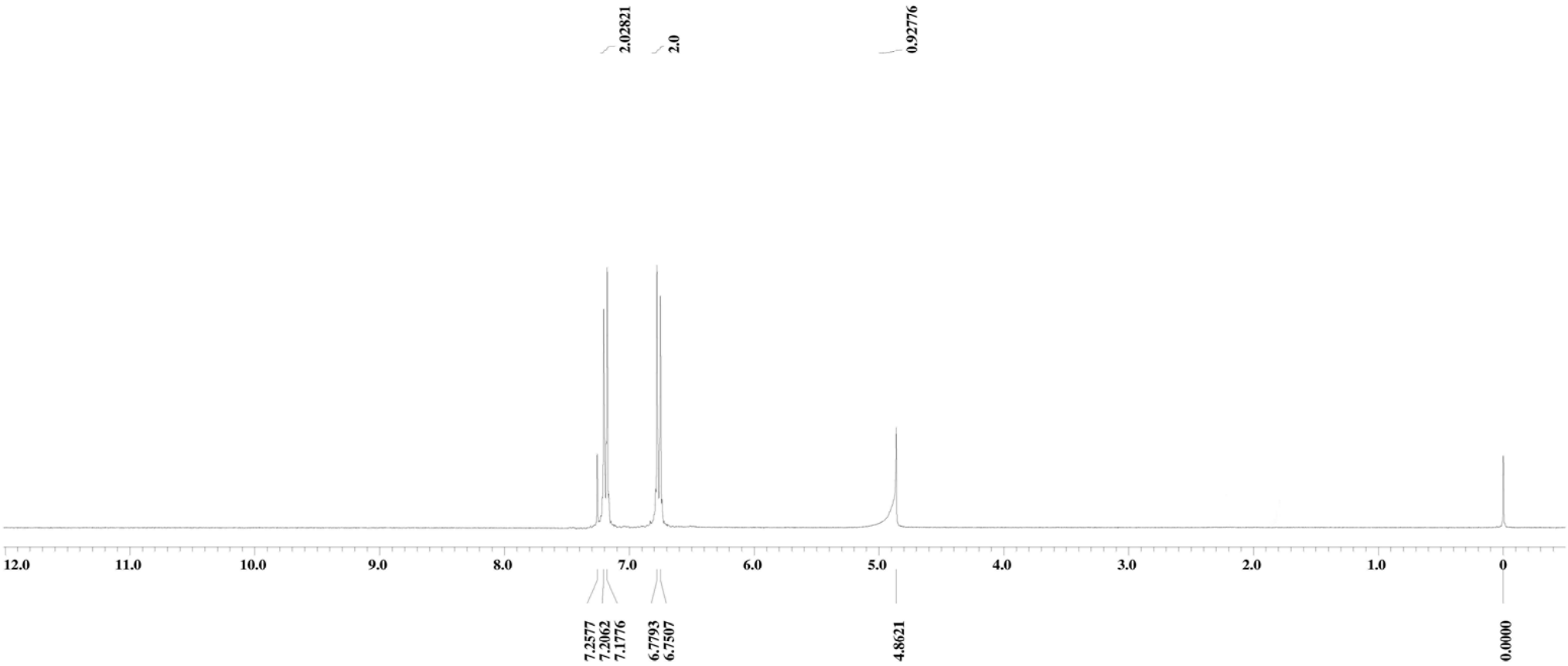

OH

2k

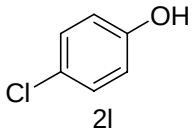

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
153.1887
134.5072
129.8321
128.8856
127.7287
126.5050
126.3424
123.6081
117.6805
109.4966
77.4207
77.0000
76.5793
X : parts per Million : 13C



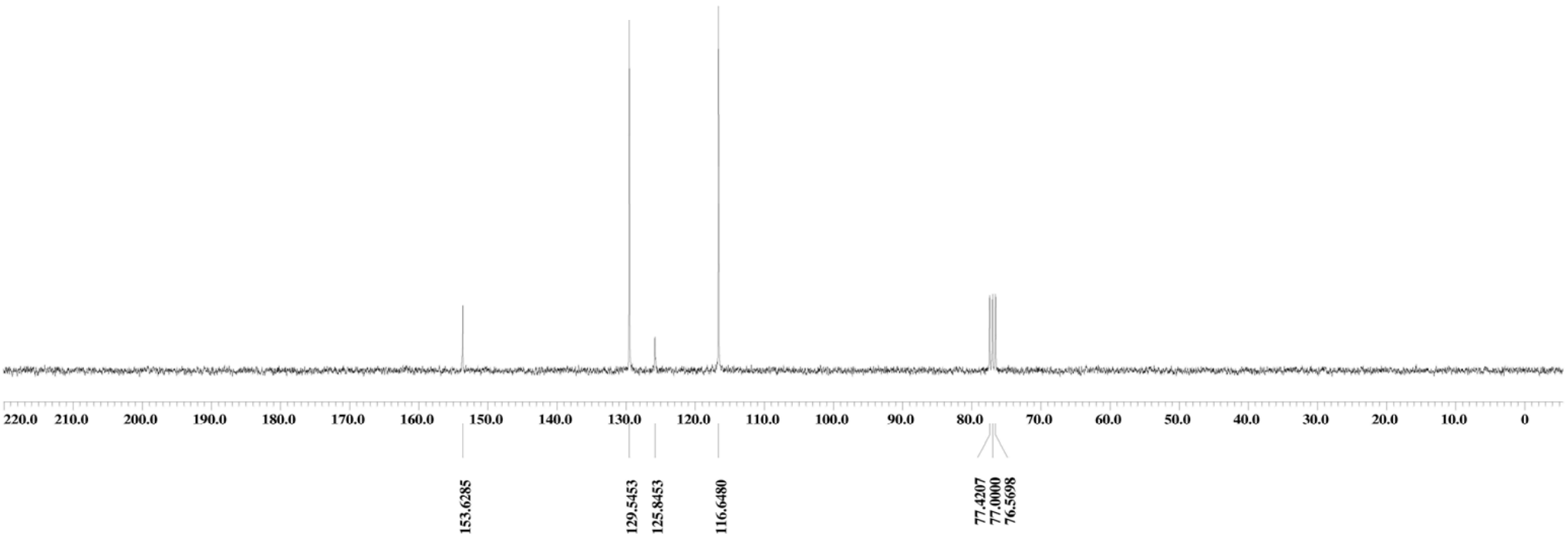
2l

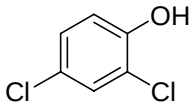


X : parts per Million : 1H

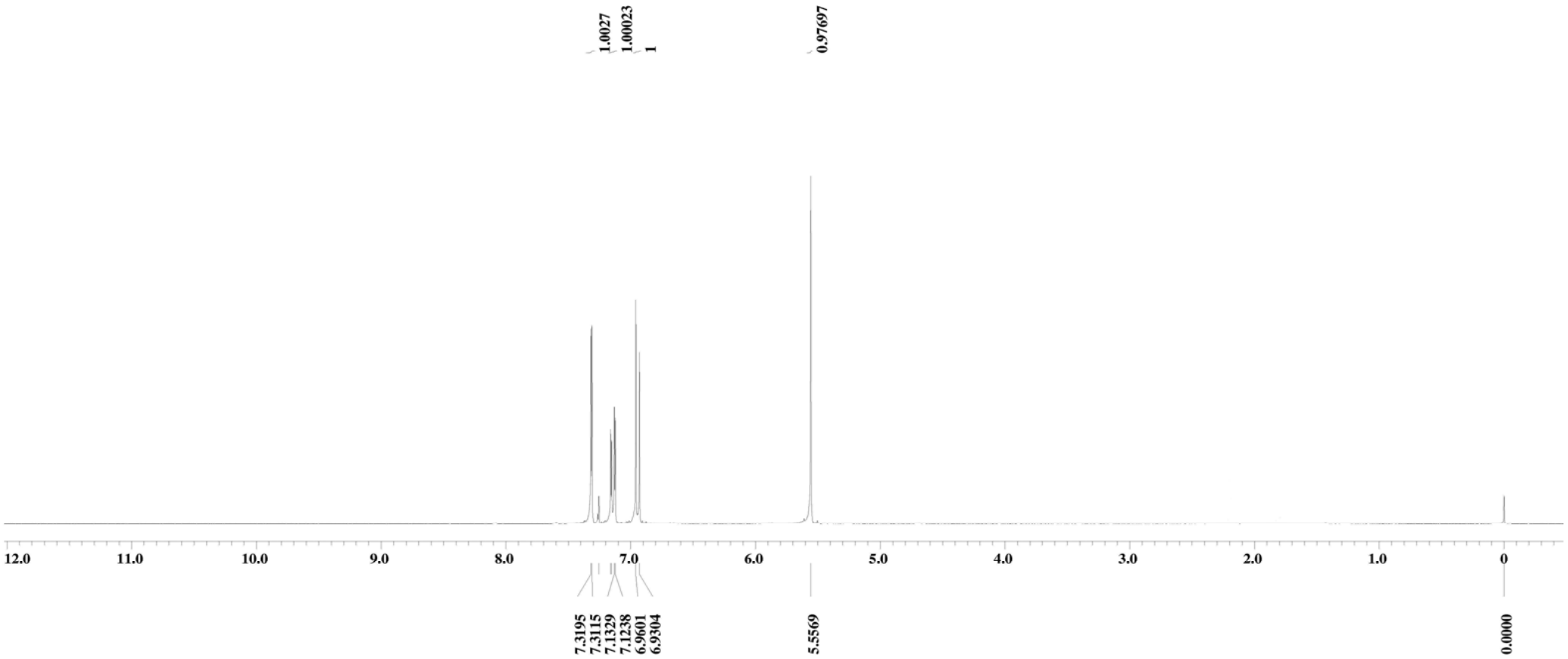

OH
Cl

2l

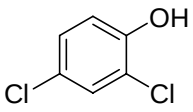

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
153.6285
129.5453
125.8453
116.6480
77.4207
77.0000
76.5698
X : parts per Million : 13C



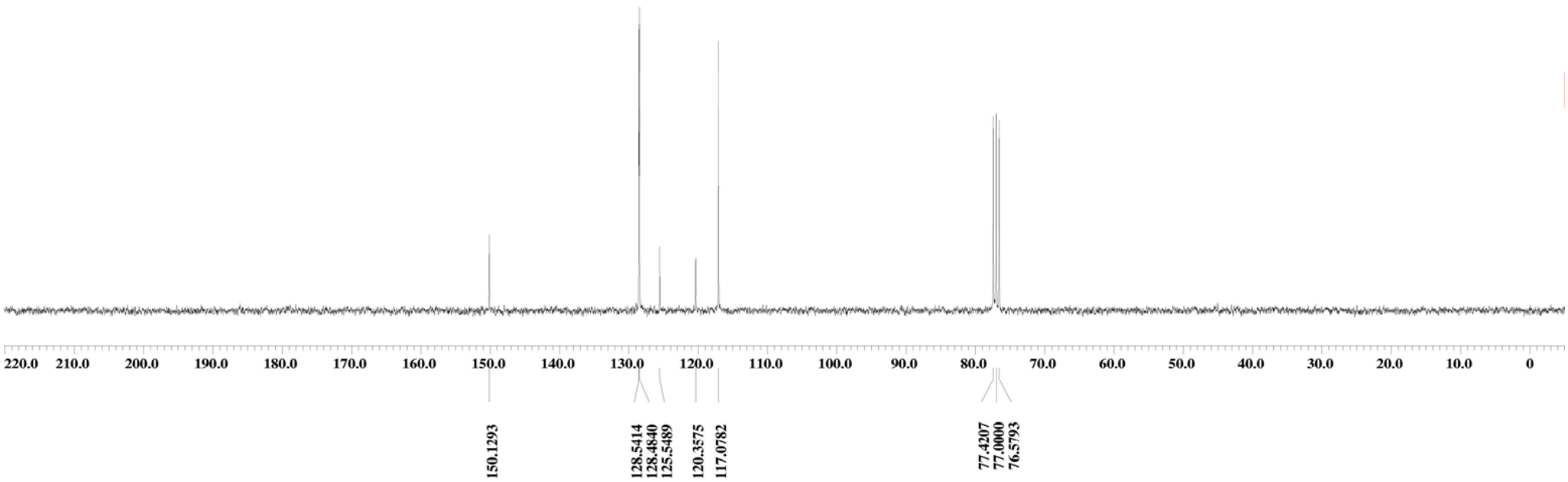
2m



X : parts per Million : 1H


OH
Cl
Cl

2m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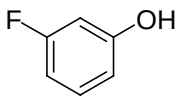
150.1293
128.5414
128.4840
125.5489
120.3575
117.0782
77.4207
77.0000
76.5793
X : parts per Million : 13C



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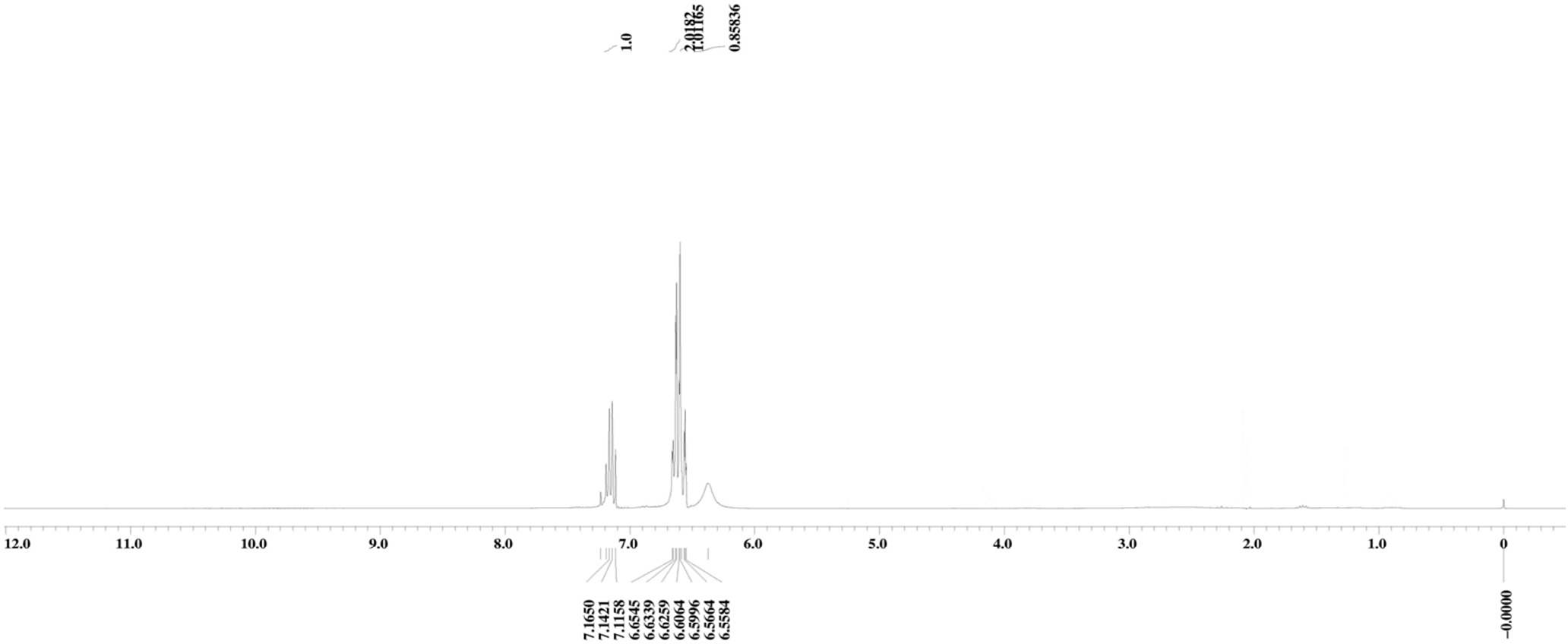
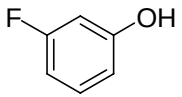
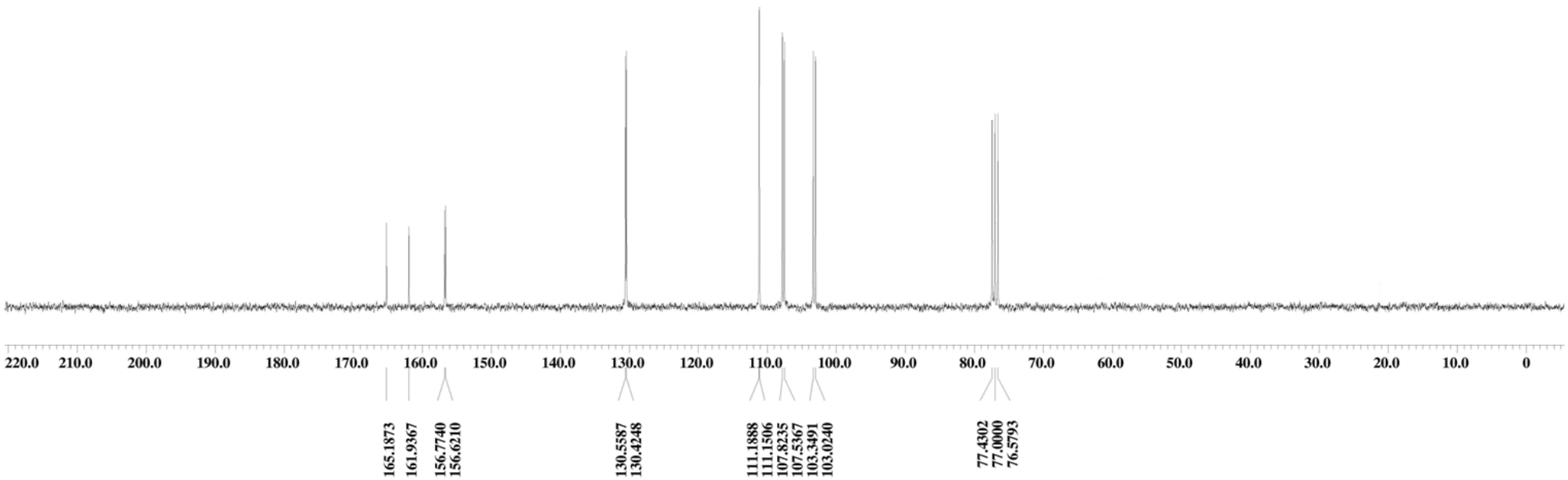


X : parts per Million : 1H


F
OH

2n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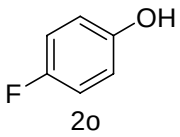
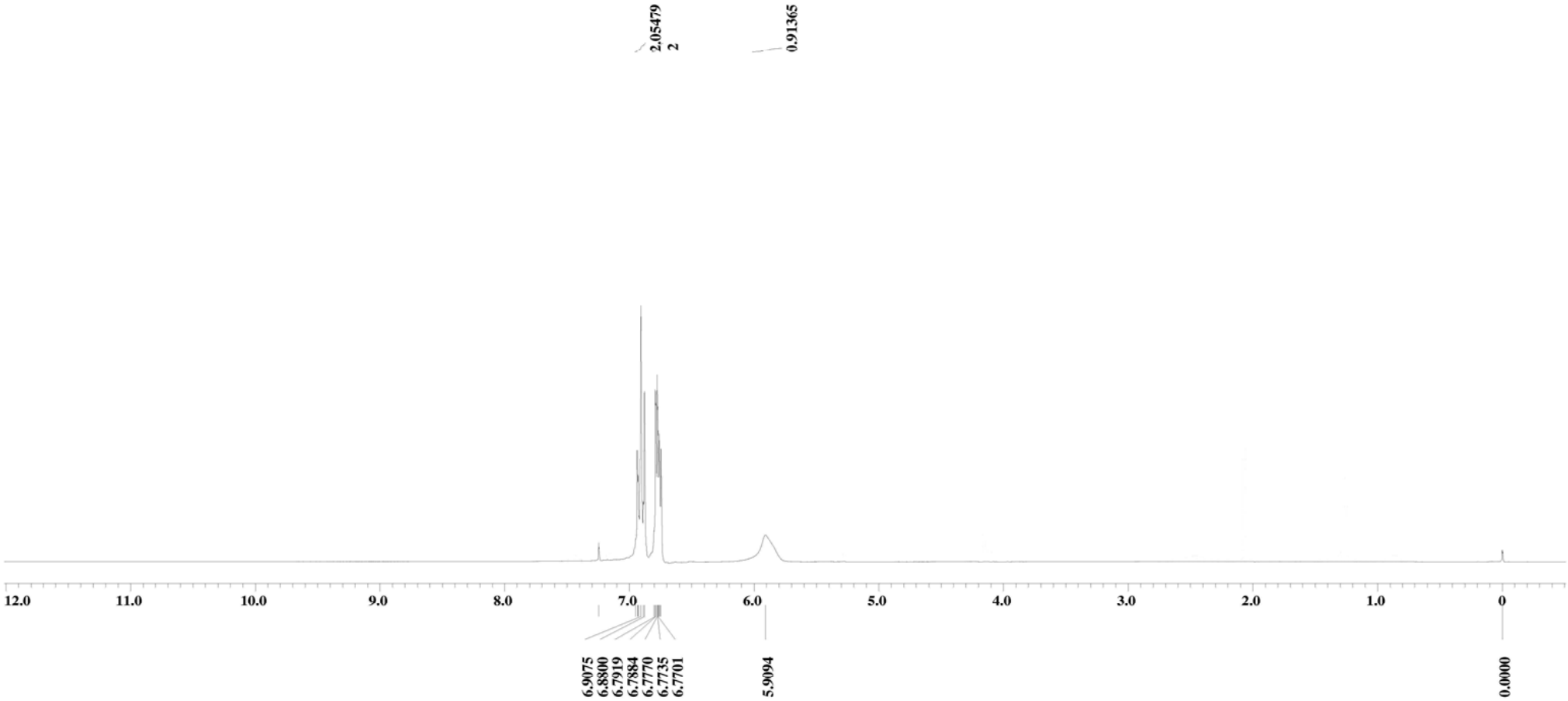
165.1873
161.9367
156.7740
156.6210
130.5587
130.4248
111.1888
111.1506
107.8235
107.5367
103.3491
103.0240
77.4302
77.0000
76.5793
X : parts per Million : 13C


OH
F

2o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2
0.91365
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
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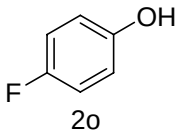
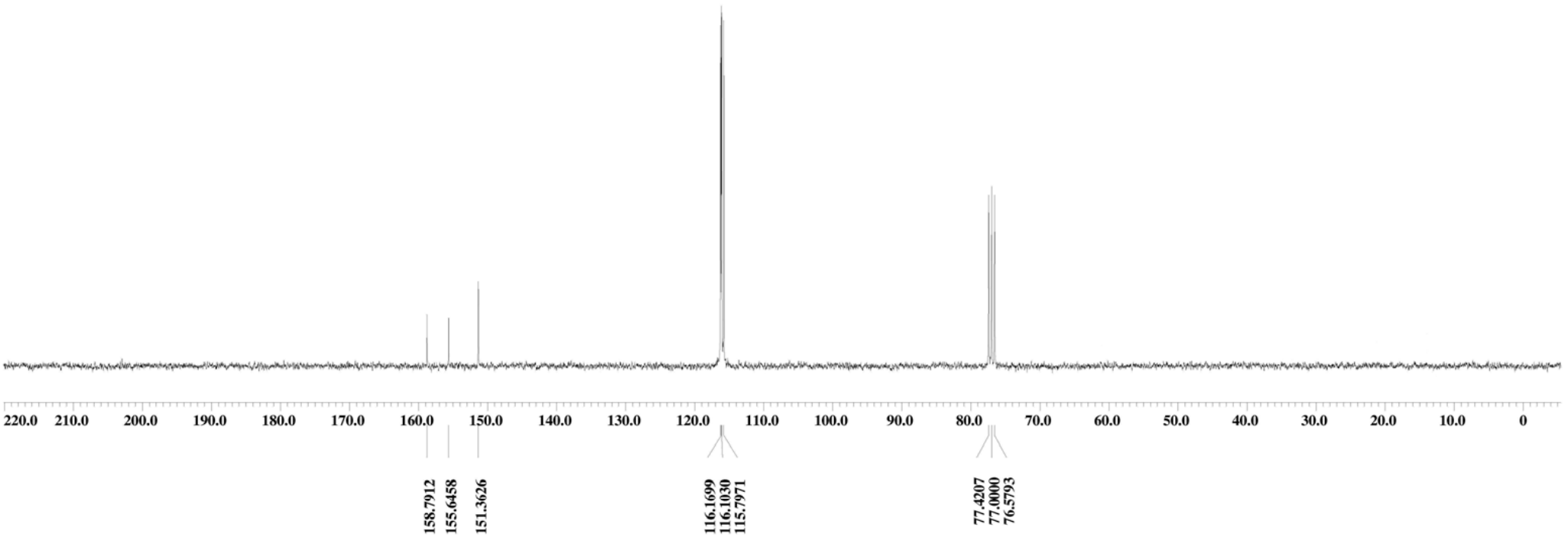
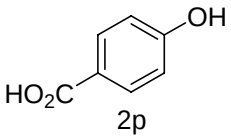
3.0
2.0
1.0
0
6.9075
6.8800
6.7919
6.7884
6.7770
6.7735
6.7701
5.9094
0.0000
X : parts per Million : 1H

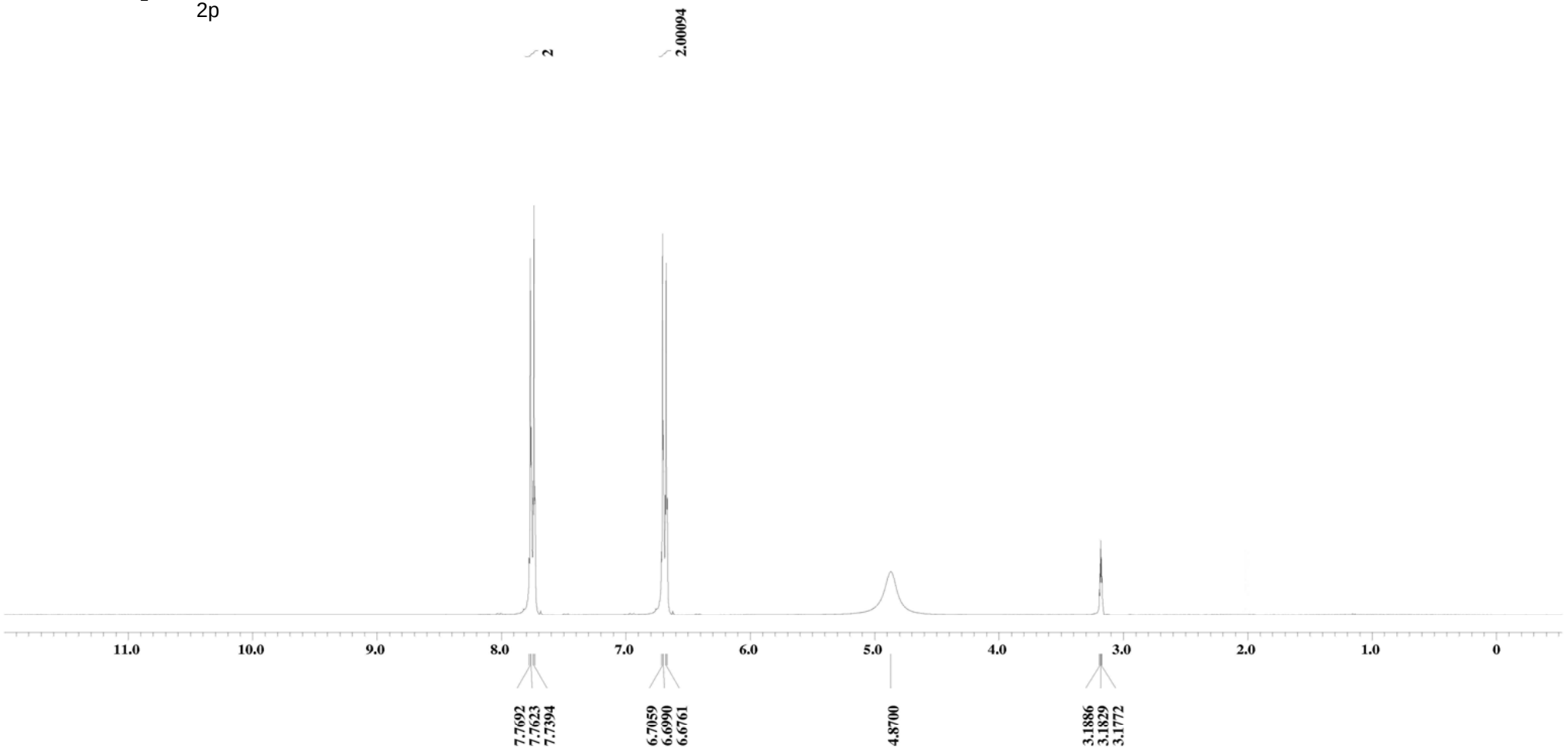

OH
F

2o

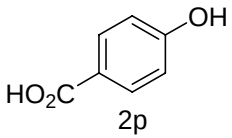

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
158.7912
155.6458
151.3626
116.1699
116.1030
115.7971
77.4207
77.0000
76.5793
X : parts per Million : 13C



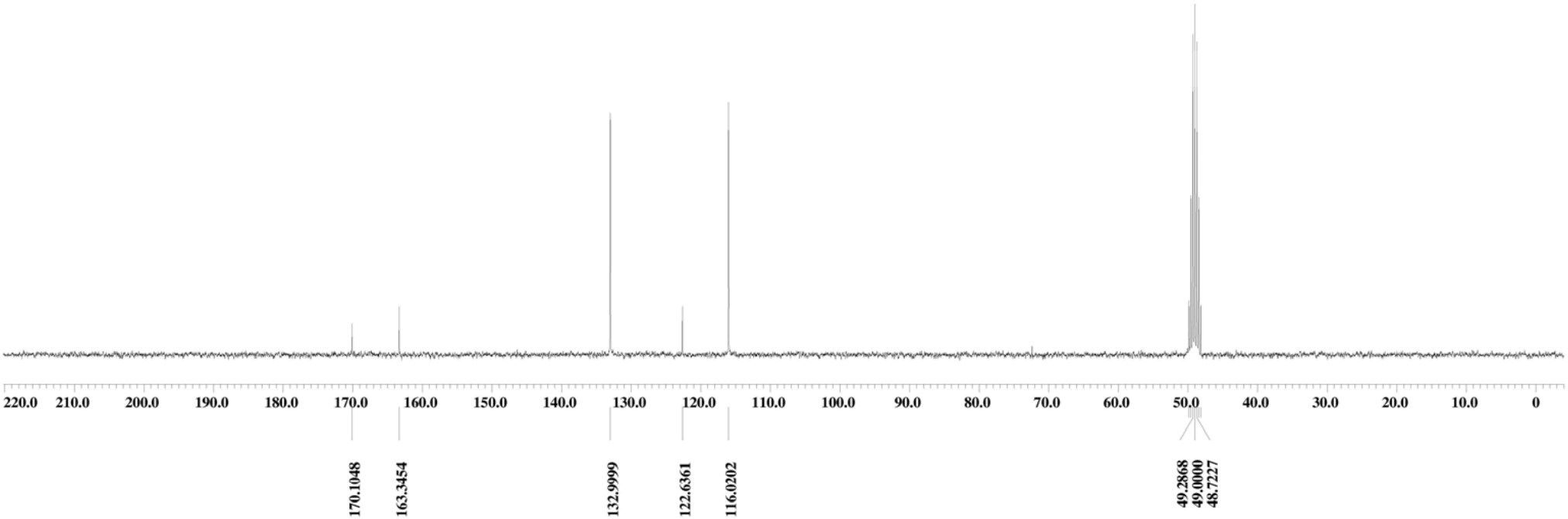
2p



X : parts per Million : 1H


OH
HO2C

2p


220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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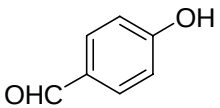
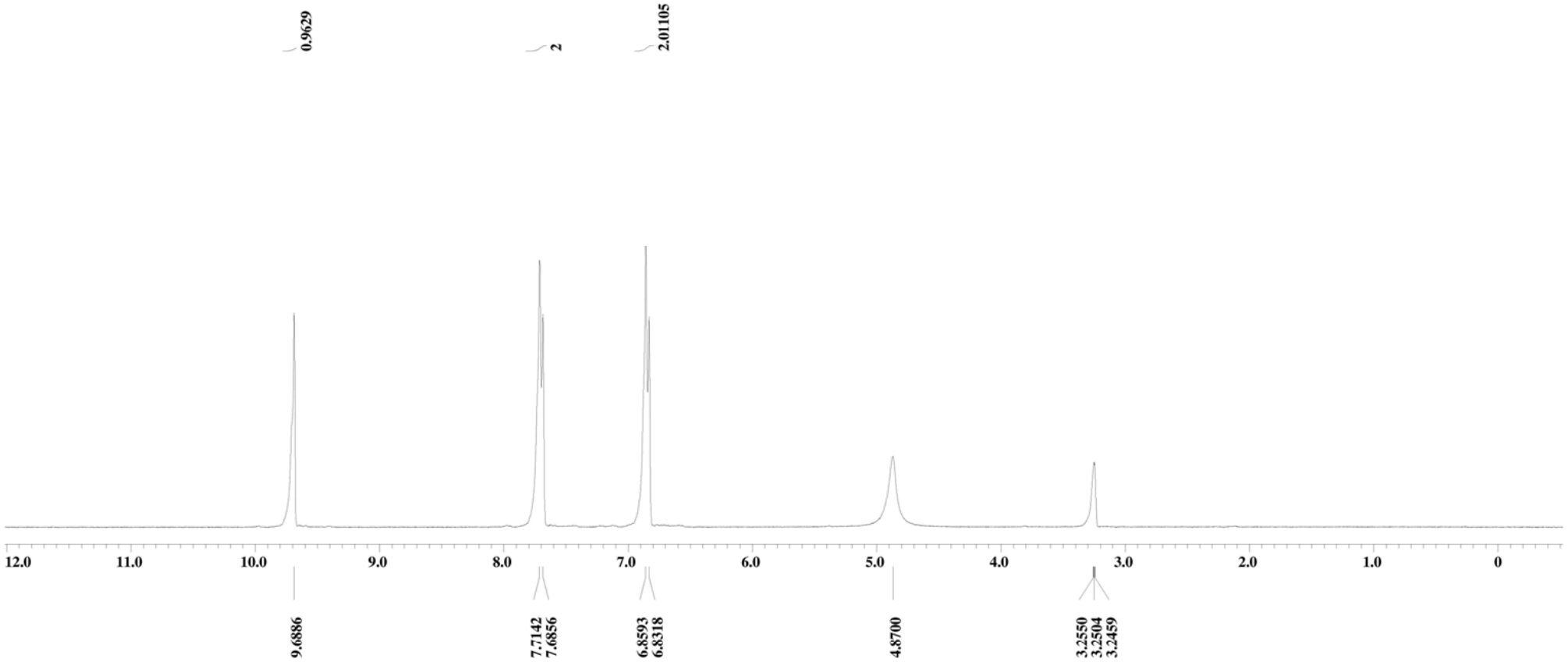
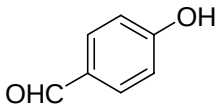
163.3454
132.9999
122.6361
116.0202
49.2868
49.0000
48.7227
X : parts per Million : 13C

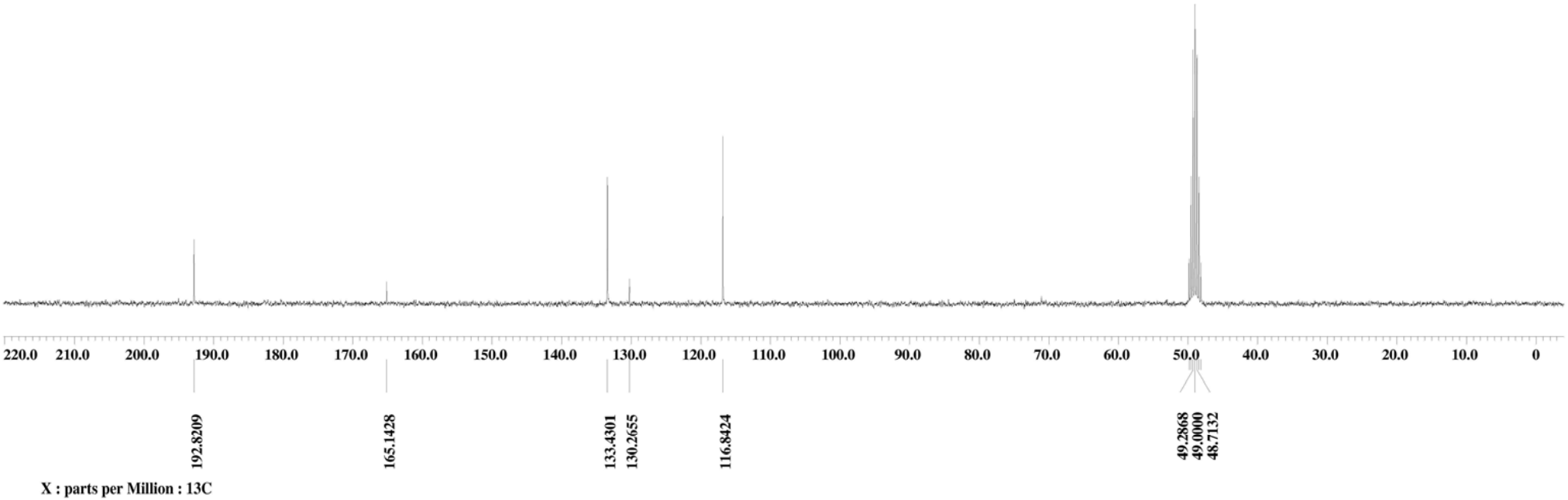

OH
OHC

2q


0.9629
2
2.01105
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.6886
7.7142
7.6856
6.8593
6.8318
4.8700
3.2550
3.2504
3.2459
X : parts per Million : 1H


OH
OHC

2q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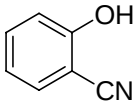
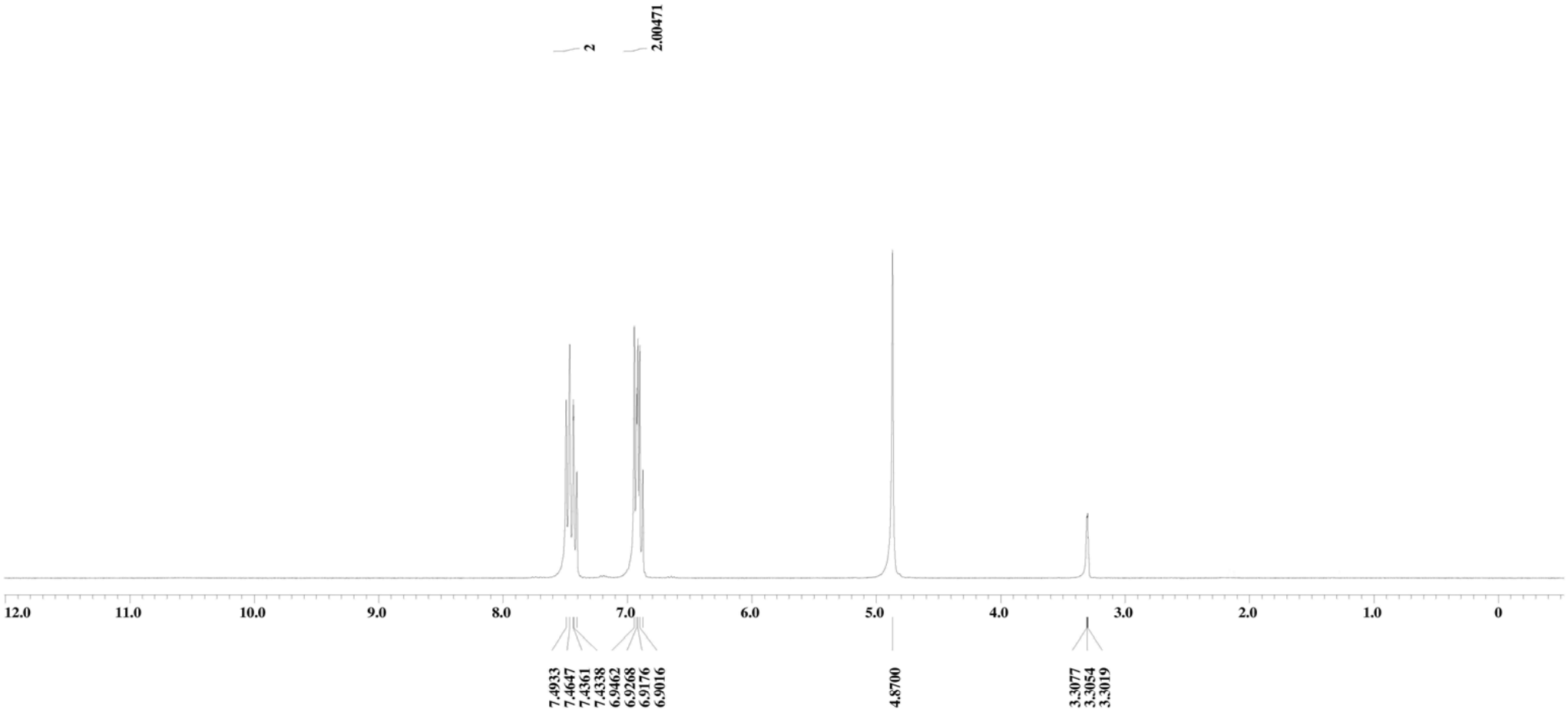
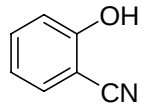
192.8209
165.1428
133.4301
130.2655
116.8424
49.2868
49.0000
48.7132
X : parts per Million : 13C



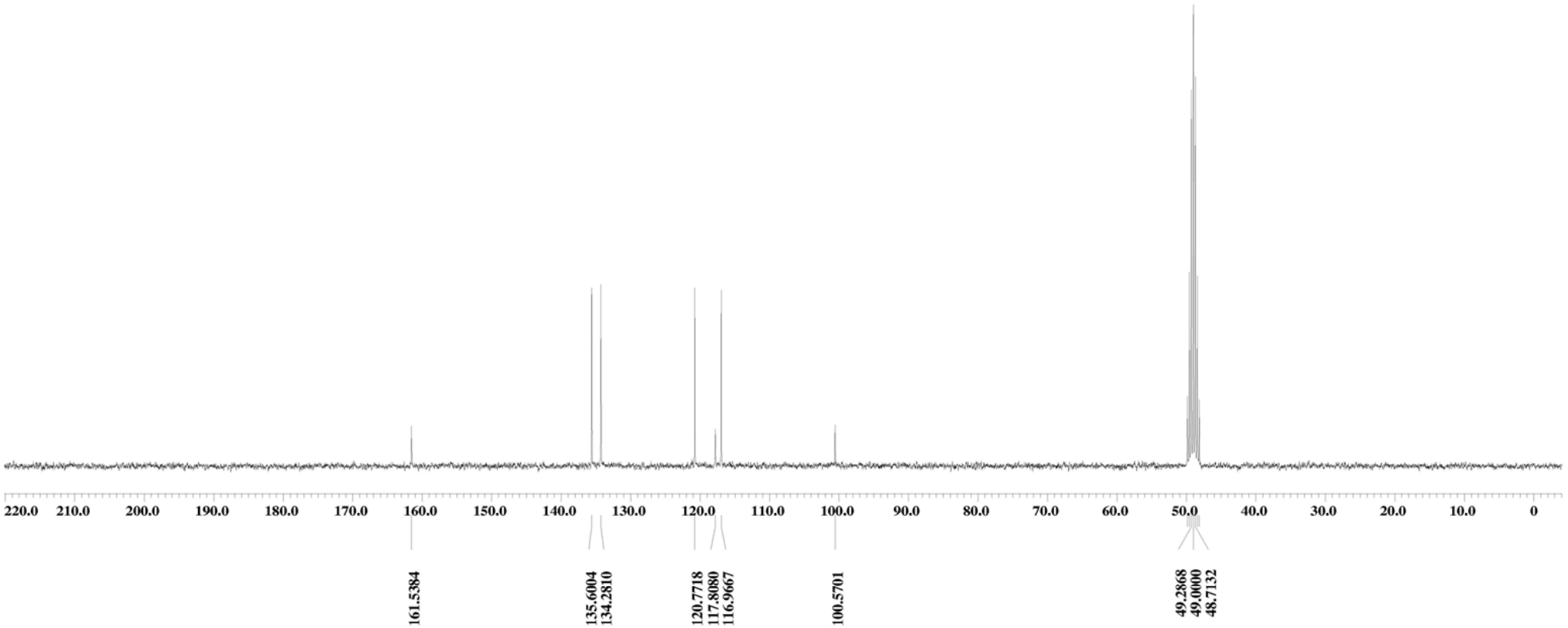
2r



X : parts per Million : 1H


OH
CN

2r


220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.5384
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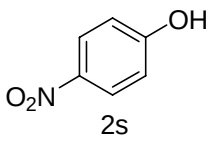
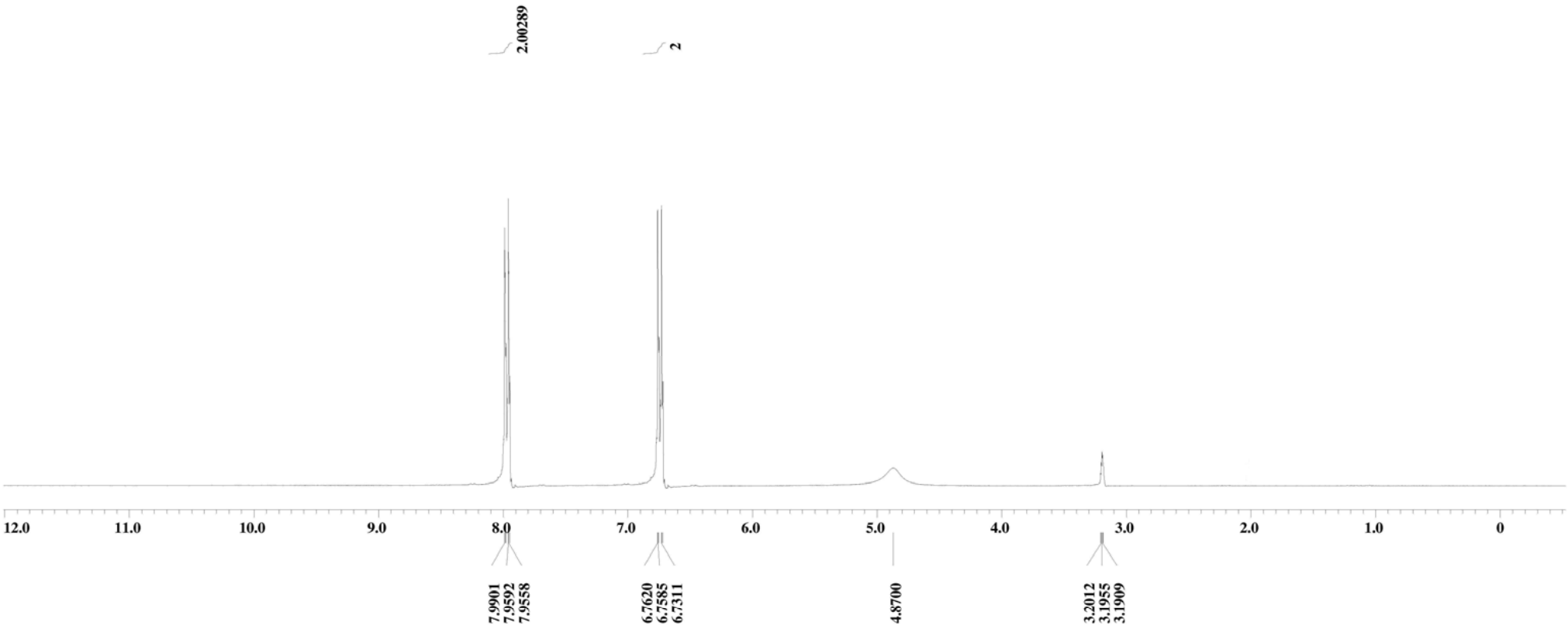
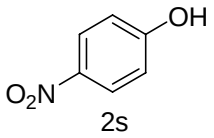
X : parts per Million : 13C



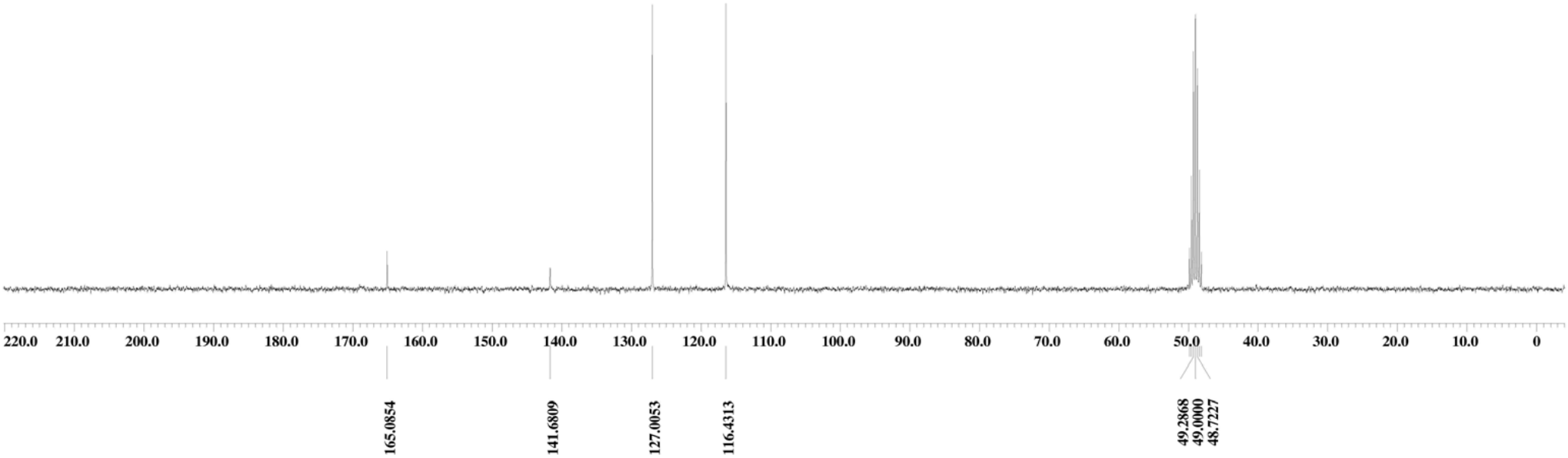
2s



X : parts per Million : 1H


OH
O_2N

2s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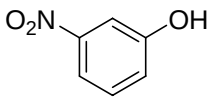
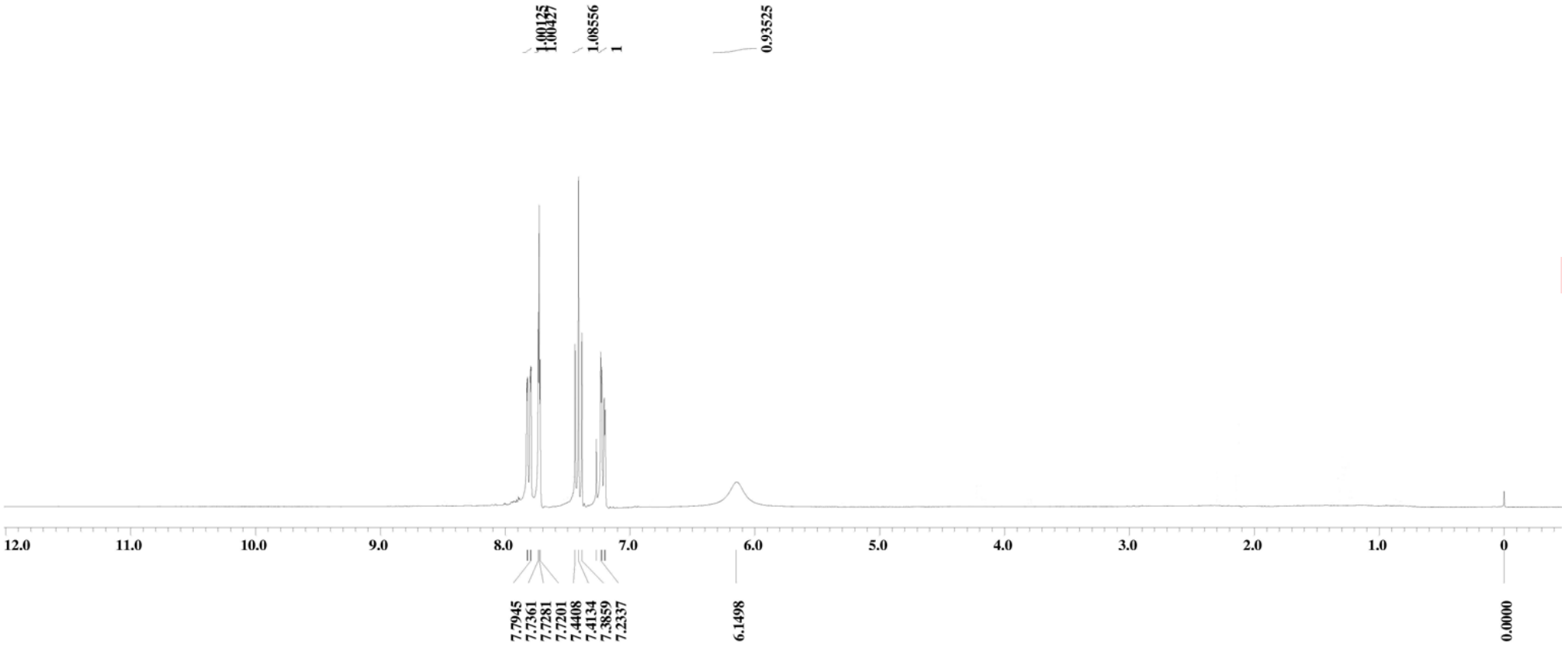
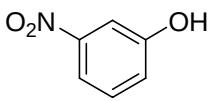
165.0854
141.6809
127.0053
116.4313
49.2868
49.0000
48.7227
X : parts per Million : 13C



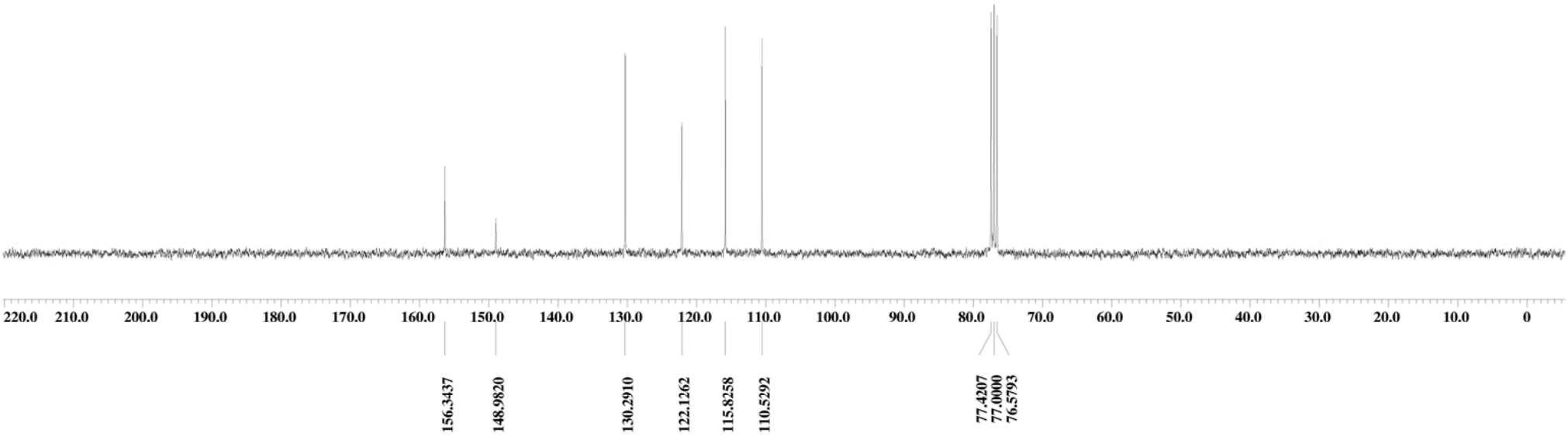
2t



X : parts per Million : 1H


O2N
OH

2t


220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
156.3437
148.9820
130.2910
122.1262
115.8258
110.5292
77.4207
77.0000
76.5793
X : parts per Million : 13C