Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

A green approach for decoration of Pd NPs on graphene nanosheets: An *in-situ* process for the reduction of C-C double bond and reusable catalyst for Suzuki cross-coupling reaction

List of the Contents

FT-IR spectral analysis

The FT-IR spectra of GO and Pd-rGO-H_2 composites material is shown in Figure S1. The peaks at 1439 and 1224 cm^{-1} of GO corresponds to the vibration of carboxyl groups and also the prominent absorption bands observed at 3130, 1732, and 1052 cm^{-1} are attributed to the stretching vibrations of O–H, C=O, C–O–C of GO, respectively. The FTIR bands observed at 1585 cm^{-1} and 1439 cm^{-1} are due to C=C stretching of aromatic rings and C–O–H bending of phenolic groups. These peaks became weak or disappeared when GO is reduced to rGO by hydrogen. This observation suggests that the oxygen functionalities present in GO such as carbonyl, hydroxyl, epoxy and carboxyl groups are substantially decreased after formation of Pd nanoparticles (Pd NPs) on to rGO sheets.

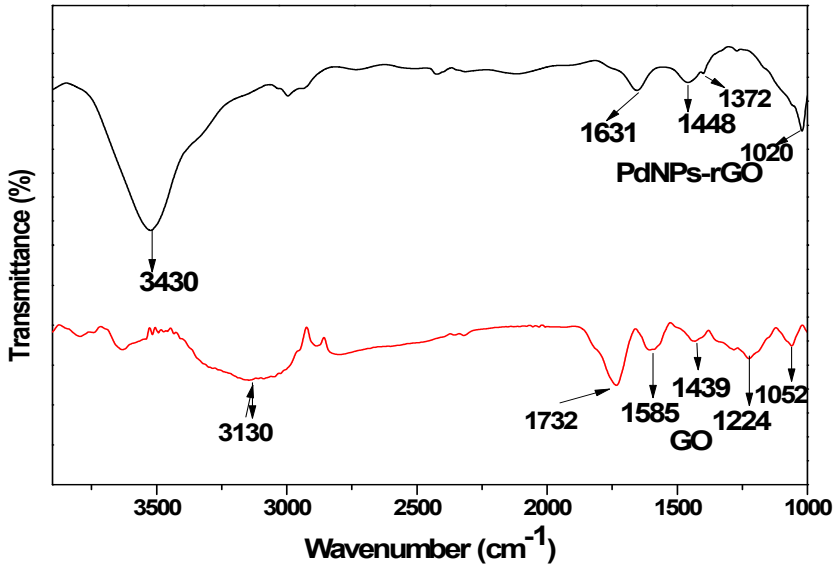


Fig. S1 FTIR spectra of the Pd-rGO-H_2 composite materials

Scanning Electron Microscope analysis

The morphology and microstructure of Pd NPs as well as its support i.e rGO sheets were investigated by Scanning electron microscope (SEM) (shown in Figure S2). The crumpled and rippled structure of GO resulting from deformation upon the exfoliation and restacking processes is partially destroyed in rGO sheets due to the reduction of large amount of oxygen containing functional groups. However, the rGO nanosheets were layered in structure, it is irregular and folded where the spherical Pd NPs are uniformly distributed.

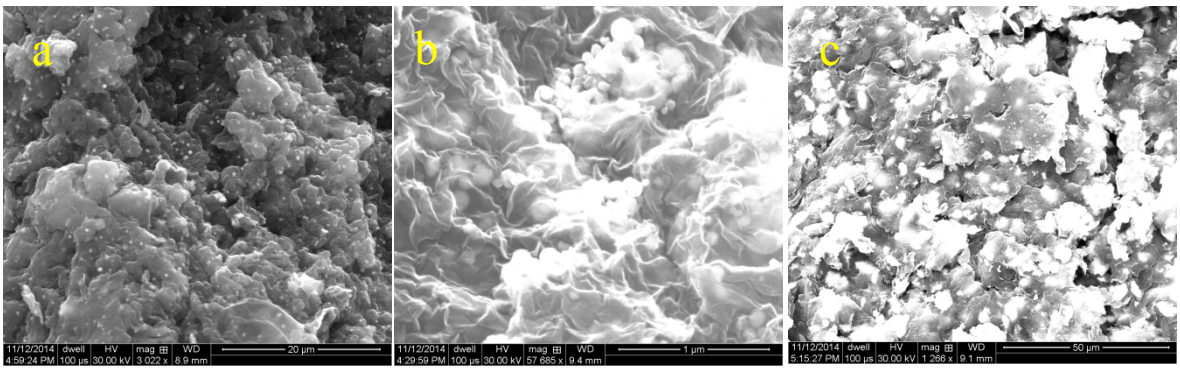


Fig. S2 SEM images of (A) Pd-rGO-H_2 (B) Pd-rGO-As and (C) Pd-rGO-Gl

Synthesis of Pd nanoparticles on rGO without addition of olefin

The Pd NPs on rGO nanosheets was synthesized by using hydrogen gas without addition of olefin to examine whether the *in-situ* process with olefin has an effect on the growth of the Pd-rGO-H_2 composite material. The synthesized composite material was characterized by XRD anlysis. As shown in Fig. S3, the prominent peaks at 2θ values of about 40.02, 46.53, 67.94, 81.85 and 86.34 are assigned to the (111), (200), (220), (311) and (222) crystallographic planes of Pd NPs with corresponding *d*-spacing value of 2.25, 1.95, 1.37, 1.17 and 1.12, respectively. The average crystallite size of the Pd NPs was

determined by using PDXL software from XRD and found to be 7.2 nm which is very close to the crystallite size of Pd-rGO-H_2 (7.6 nm). Moreover, all the diffraction peak values along with the *d*-spacing values are compared with the Pd-rGO-H_2 and found almost same. The XRD analysis clearly suggests that there is no significant effect of catalytic process on the growth of Pd-rGO-H_2 nanohybrids.

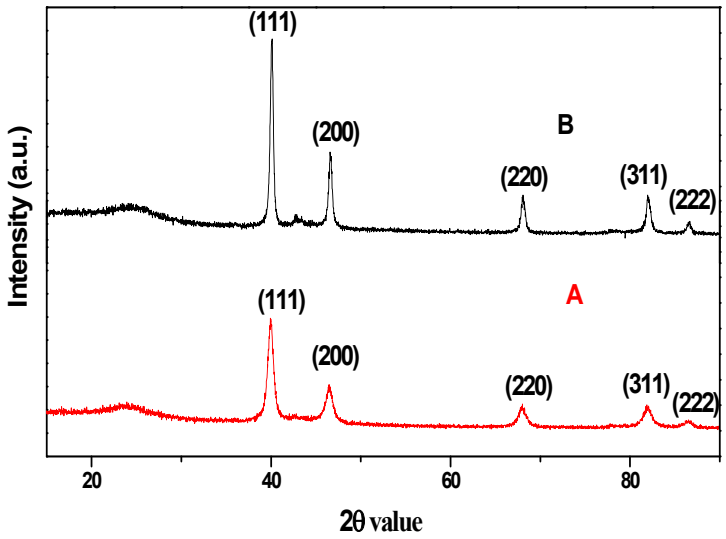
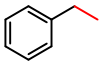


Fig. S3 XRD pattern of Pd NPs on rGO nanosheets: (A) *In situ* synthesis Pd-rGO-H_2 composite along with olefin, (B) *Ex situ* synthesis of Pd-rGO-H_2 composite without addition of olefin

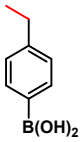
Analytical data

Ethylbenzene, **4a**:



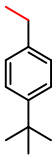
[85.8 mg, 81%, Liquid]; ^{1}H NMR (500 MHz, $CDCl_3$): δ= 7.07-7.44 (m, 5H), 2.67 (q, *J*=7.6 Hz, 2H), 1.26 (t, *J*=7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 144.1, 128.2, 127.7, 125.5, 28.7, 15.5; IR ($CHCl_3$): 2964, 2931, 2870, 1519, 1460, 1363, 1020 cm^{-1}.

(4-Ethylphenyl)boronic acid, **4b**:



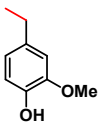
[118 mg, 79%, White solid, mp 152-157 ^{o}C]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 8.15 (d, *J*=7.7 Hz, 2H), 7.33 (d, *J*=7.7 Hz, 2H), 2.73 (q, *J*=7.7 Hz, 2H), 1.29 (t, *J*=7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 149.1, 135.8, 133.7, 127.6, 29.2, 15.4; IR ($CHCl_3$): 3339, 2966, 1610, 1408, 1368, 1342 cm^{-1}; MS (EI) m/z: 117 $(M-H_2O)^{+}$

1-(*tert*-Butyl)-4-ethylbenzene, **4c:**



[133 mg, 82%, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.31 (d, *J*=8.1 Hz, 2H), 7.14 (d, *J*=8 Hz, 2H), 2.62 (q, *J*=7.6 Hz, 2H), 1.31 (s, 9H), 1.23 (t, *J*=7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 148.5, 141.3, 127.7, 125.4, 34.5, 31.7, 28.5, 15.7; IR ($CHCl_3$): 2963, 2932, 2870, 1517, 1461, 1363, 1019, 828, 772 cm^{-1}

4-Ethyl-2-methoxyphenol, **4d**:

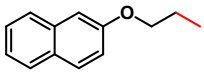


[129 mg, 85 %, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 6.82 (d, *J*=8.3 Hz, 1H), 6.68 (s, 1H), 6.67 (d, *J*=8.3 Hz, 1H), 5.41 (br s, 1H), 3.87 (s, 3H), 2.51 (t, *J*=7.6 Hz, 2H), 1.59 (m, 2H), 0.93 (t, *J*=7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 146.3, 143.5, 134.7, 120.9, 114.1, 111.1, 55.8, 37.8, 24.8, 13.8; IR ($CHCl_3$): 3448, 2958, 2930, 2870, 1606, 1513, 1267, 1234, 1151, 1123, 1034, 816, 795 cm^{-1}

1-Propoxynaphthalene, **4e**:

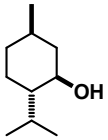
[97 mg, 52%, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 8.3 (d, *J*=9.2 Hz, 1H), 7.78 (d, *J*=8.9 Hz, 1H), 7.3-7.5 (m, 4H), 6.79 (d, *J*=7.1 Hz, 1H), 4.1 (t, *J*=6.4 Hz, 2H), 1.94 (m, 2H), 1.37 (t, *J*=7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 155.0, 138.6, 134.6, 127.5, 126.4, 126.1, 125.2, 122.2, 120.1, 104.7, 69.7, 22.8, 10.9; IR ($CHCl_3$): 3053, 2963, 1582, 1405, 1389, 1240, 1072, 79l0 cm^{-1}

2-Propoxynaphthalene, **4f**:



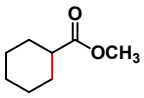
[91 mg, 49 %, Liquid];^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.36-7.52 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 157.1, 134.7, 129.3, 128.9, 127.6, 126.7, 126.3, 123.5, 119.1, 106.6, 69.5, 22.6, 10.7; IR ($CHCl_3$): 2963, 2934, 1629, 1600, 1510, 1465, 1389, 1258, 1217, 1182, 1119, 985, 836, 745 cm^{-1}

(-) Menthol, 4g:



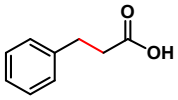
[144 mg, 92%, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 3.41 (dt, J_1=4.2, J_2=10.4 Hz, 1H), 2.17 (m, 1H), 1.96 (br d, *J*=11.9 Hz, 1H), 1.52-1.75 (m, 3H), 1.41 (br s, 1H), 0.92 (dd, J_1=5.0, J_2=6.4 Hz, 6H), 0.81 (d, *J*=6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 71.6, 50.1, 45.1, 34.5, 31.6, 25.8, 23.2, 22.2, 21.0, 16.1; IR ($CHCl_3$): 3351, 2954, 2921, 2870, 1455, 1368, 1044, 1024, 771 cm^{-1}

Methyl cyclohexanecarboxylate, 4h:



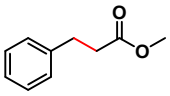
[53 mg, 37 %, Gummy]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 2.25 (br s, 1H), 2.05 (s, 3H), 1.60-1.87 (m, 4H), 1.02-1.32 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 212.2, 51.4, 28.4, 27.8, 25.8, 25.6; IR ($CHCl_3$): 2930, 2855, 1709, 1449, 1371, 1351, 1167 cm^{-1}

3-Phenylpropanoic acid, **4i**:



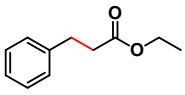
[120 mg, 80%, Gummy];^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.07-7.29 (m, 5H), 2.88 (t, *J*=7.7 Hz, 2H), 2.61 (t, *J*=7.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 179.0, 140.2, 128.6, 128.3, 126.4, 35.6, 30.6; IR ($CHCl_3$): 3029, 2927, 1709, 1496, 1454, 1412, 1293, 699 cm^{-1}

Methyl 3-phenylpropanoate, **4j**:



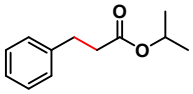
[135 mg, 82%, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.99-7.49 (m, 5H), 3.67 (s, 3H), 2.95 (t, *J*=7.8 Hz, 2H), 2.63 (t, *J*=7.8 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 173.3, 140.5, 128.5, 128.3, 126.3, 51.6, 35.7, 30.9; IR ($CHCl_3$): 3028, 2952, 1739, 1454, 1437, 1196, 1163, 1029, 751, 700 cm^{-1}

Ethyl 3-phenylpropanoate, **4k**:



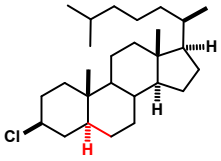
[155 mg, 87 %, Yellow solid,]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 6.92-7.49 (m, 5H), 4.12 (q, *J*=7.1 Hz, 2H), 2.95 (t, *J*=7.8 Hz, 2H), 2.62 (t, *J*=7.8 Hz, 2H), 1.23 (t, *J*=7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 172.9, 140.6, 128.5, 128.3, 126.2, 60.4, 35.9, 31.0, 14.2; IR ($CHCl_3$): 3029, 2982, 2934, 1735, 1455, 1373, 1295, 1180, 1161, 1039, 752, 699 cm^{-1}

Isopropyl 3-phenylpropanoate, **4l**:



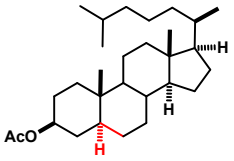
[183 mg, 95%, Liquid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.19-7.30 (m, 5H), 5.0 (m, 1H), 2.94 (t, *J*=7.8 Hz, 2H), 2.59 (t, *J*=7.8 Hz, 2H), 1.20 (d, *J*=6.2 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 172.4, 140.6, 128.4, 128.3, 126.2, 67.6, 36.2, 31.1, 21.8; IR ($CHCl_3$): 3070.5, 2957.5, 1719.1, 1606.8, 1520.2, 1467, 1298, 743 cm^{-1}

3β-Chloro-5α-cholestane, 4m:



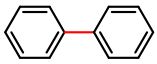
[387 mg, 95%, White solid,]; Spectroscopic data for major isomer; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 3.86 (m, 1H), 0.87 (br s, 6H), 0.84 (d, *J*=5.7 Hz, 6H), 0.64 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 60.3, 56.5, 56.3, 54.2, 46.8, 42.6, 40.0, 39.7, 39.5, 38.7, 36.2, 35.8, 35.4, 35.3, 33.2, 32.0, 28.5, 28.3, 28.1, 24.2, 23.9, 22.9, 22.6, 21.2, 18.7, 12.3, 12.1; IR ($CHCl_3$): 2930, 2848, 1466, 1446, 1167, 805, 756 cm^{-1}

3β-Acetoxy-5α-cholestane, 4n:



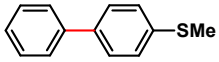
[422 mg, 98%, White solid]; Spectroscopic data for major isomer; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 4.68 (m, 1H), 2.01 (s, 3H), 0.87 (br s, 6H), 0.83 (d, *J*=10.4 Hz, 6H), 0.64 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 170.6, 73.8, 56.4, 56.3, 54.3, 44.7, 42.6, 40.0, 39.6, 36.8, 36.2, 35.8, 35.5, 34.1, 32.0, 28.6, 28.3, 28.0, 27.5, 24.2, 23.9, 22.8, 22.6, 21.5, 21.2, 18.7, 12.2, 12.1; IR ($CHCl_3$): 2935, 2915, 2851, 1729, 1468, 1368, 1264, 1042, 1029, 772 cm^{-1}

1,1'-Biphenyl, 5a:



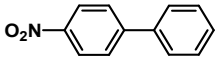
[148 mg, 96 %, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (d, *J*=7.3 Hz, 4H), 7.41 (t, *J*=7.5 Hz, 4H), 7.32 (d, *J*=7.1 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 141.4, 128.9, 127.4, 127.3; IR ($CHCl_3$): 2925, 1429, 1216 cm^{-1}.

1,1'-Biphenyl]-4-yl(methyl)sulfane, 5b:



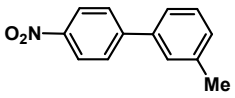
[190 mg, 95%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.47-7.58 (m, 4H), 7.41 (t, *J*=7.5 Hz, 2H), 7.27-7.35 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 140.6, 138.1, 137.6, 128.9, 127.5, 127.3, 127.0, 126.9, 15.9; IR ($CHCl_3$): 2983, 2917, 1478, 1215, 1097, 823, 754 cm^{-1}.

4-Nitro-1,1'-biphenyl, 5c:



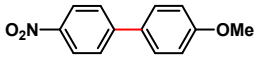
[191 mg, 96%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 8.17 (d, *J*=8.6 Hz, 2H), 7.61 (d, *J*=8.6 Hz, 2H), 7.51 (d, *J*=6.9 Hz, 2H), 7.30-7.43 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 147.6, 147.1, 138.7, 129.2, 128.9, 127.8, 127.4, 124.1; IR ($CHCl_3$): 2839, 1597, 1575, 1480, 1352, 1079, 912, 741 cm^{-1}.

3-Methyl-4'-nitro-1,1'-biphenyl, 5d:



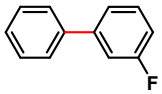
[204 mg, 96%, light yellow solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 8.17 (d, *J*=8.3 Hz, 2H), 7.61 (d, *J*=8.3 Hz, 2H), 7.26-7.38 (m, 3H), 7.16 (d, *J*=6.6 Hz, 1H), 2.34 (br s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 147.8, 147.0, 138.9, 138.7, 129.7, 129.1, 128.1, 127.8, 124.5, 124.1, 21.5; IR ($CHCl_3$): 2923, 1596, 1516, 1346, 1107, 854, 843, 750 cm^{-1}.

4-Methoxy-4'-nitro-1,1'-biphenyl, 5e:



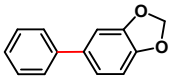
[215 mg, 94%, yellow solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 8.24 (d, *J*=8.7 Hz, 2H), 7.67 (d, *J*=8.7 Hz, 2H), 7.57 (d, *J*=8.7 Hz, 2H), 7.01 (d, *J*=8.7 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 160.5, 147.2, 146.5, 131.0, 128.6, 127.1, 124.1, 114.6, 55.4; IR ($CHCl_3$): 3019, 2930, 2836, 1600, 1509, 1344, 1016, 757 cm^{-1}.

3-Fluoro-1,1'-biphenyl, 5f:



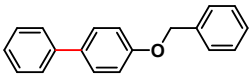
[160 mg, 93%), white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (d, *J*=7.3 Hz, 2H), 7.43 (t, *J*=7.3 Hz, 2H), 7.32-7.39 (m, 3H), 7.27 (d, *J*=9.9 Hz, 1H), 6.96-7.08 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 163.3 (d, *J*=245 Hz), 143.5 (d, *J*=7.8 Hz), 140.0 (d, *J*=2.1 Hz), 130.2 (d, *J*=8.4 Hz), 128.9, 127.9, 127.1, 122.8 (d, *J*=2.7 Hz), 114.1 (d, *J*=21.5 Hz) IR ($CHCl_3$): 3032, 2926, 1482, 1429, 1216, 728 cm^{-1}.

5-Phenylbenzo[d][1,3]dioxole, 5g:



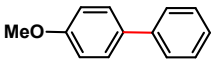
[188 mg, 95%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.50 (d, *J*=7.7 Hz, 2H), 7.39 (t, *J*=7.5 Hz, 2H), 7.31 (d, *J*=7.2 Hz, 1H), 7.05 (d, *J*=8.1 Hz, 2H), 6.86 (d, *J*=7.8 Hz, 1H), 5.97 (br s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 148.2, 147.1, 140.9, 135.6, 128.8, 127.0, 126.9, 120.7, 108.6, 107.7, 101.2; IR ($CHCl_3$): 3063, 3032, 2892, 1601, 1509, 1478, 1429, 1224, 1039, 937 cm^{-1}.

4-(Benzyloxy)-1,1'-biphenyl, 5h:



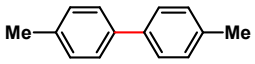
[139 mg, 92%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.52 (t, *J*=7.7 Hz, 4H), 7.26-7.46 (m, 8H), 7.03 (d, *J*=8.5 Hz, 2H), 5.07 (s, 2H; ^{13}C NMR (75 MHz, $CDCl_3$): δ= 158.4, 140.8, 137.1, 134.1, 128.8, 128.7, 128.2, 128.1, 127.5, 126.8, 126.7, 115.2; IR ($CHCl_3$): 2924, 2907, 2866, 1454, 907, 734 cm^{-1}.

4-Methoxy-1,1'-biphenyl, 5i:



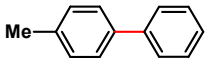
[141 mg, 95%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.46 (t, *J*=7.3 Hz, 4H), 7.33 (t, *J*=7.5 Hz, 2H), 7.22 (t, *J*=7.3 Hz, 3H), 6.90 (d, *J*=8.6 Hz, 2H), 3.76 (br s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 159.2, 140.8, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.4; IR ($CHCl_3$): 2959, 2925, 1608, 1450, 1270, 1035, 910, 833, 760 cm^{-1}.

4,4'-Dimethyl-1,1'-biphenyl, 5j:

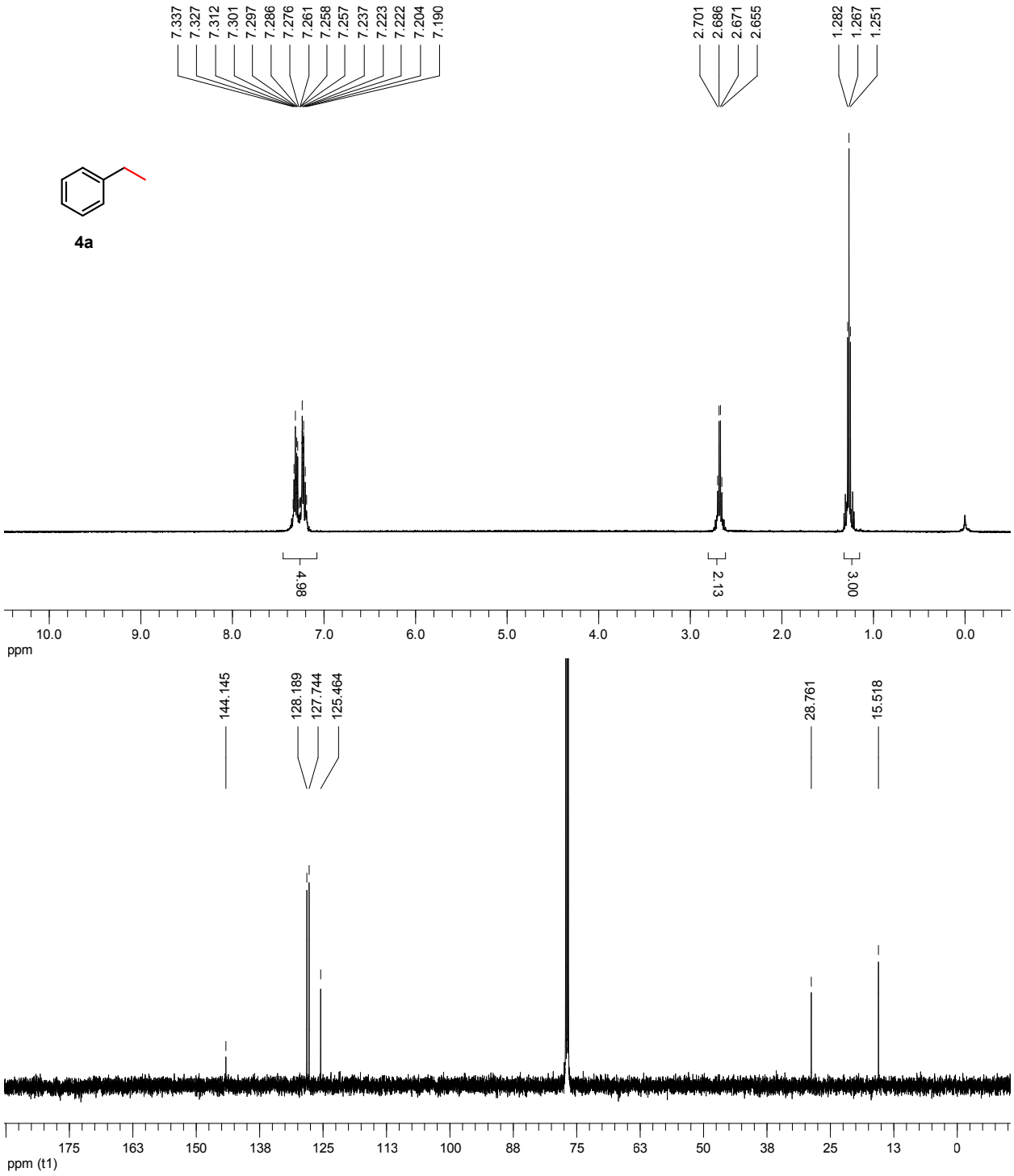


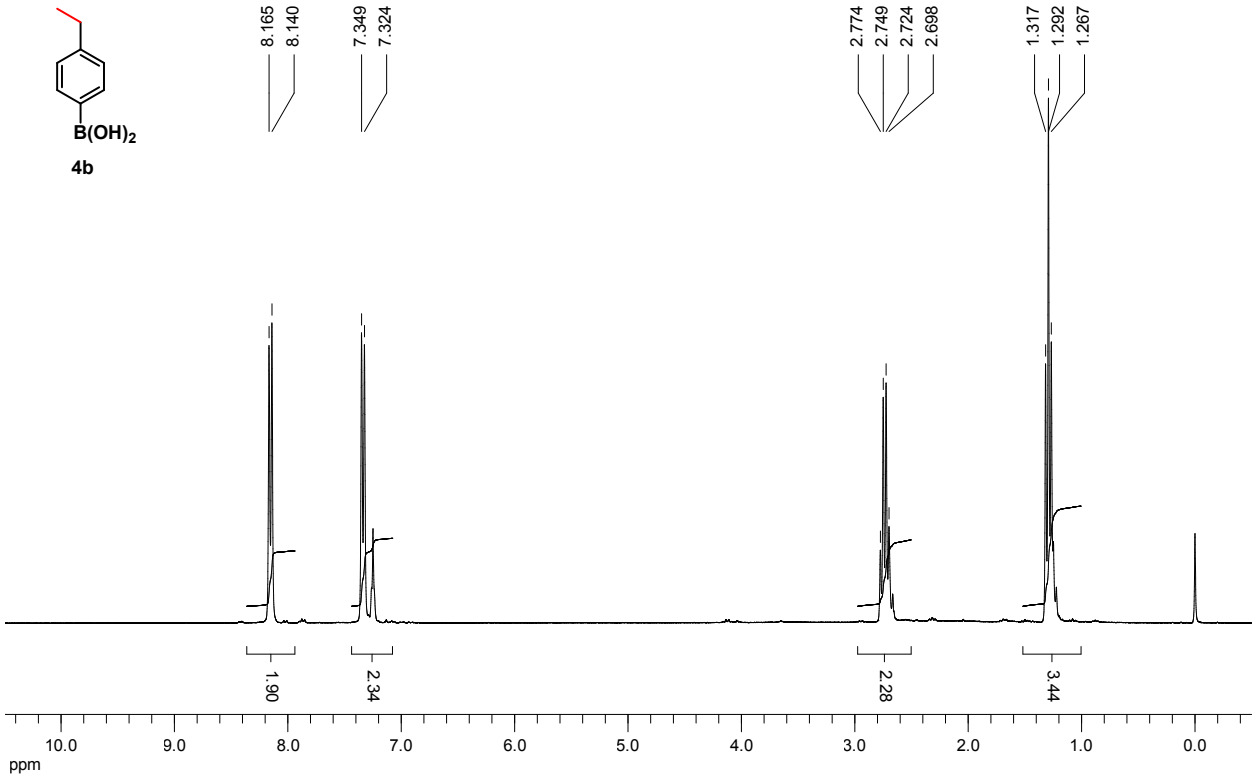
[171 mg, 94%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.47 (d, *J*=7.8 Hz, 4H), 7.23 (d, *J*=8.0 Hz, 4H), 2.38 (br s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ= 138.3, 136.7, 129.4, 126.8, 21.1; IR ($CHCl_3$): 3024, 2923, 2855, 1501, 1216, 908, 803, 758 cm^{-1}.

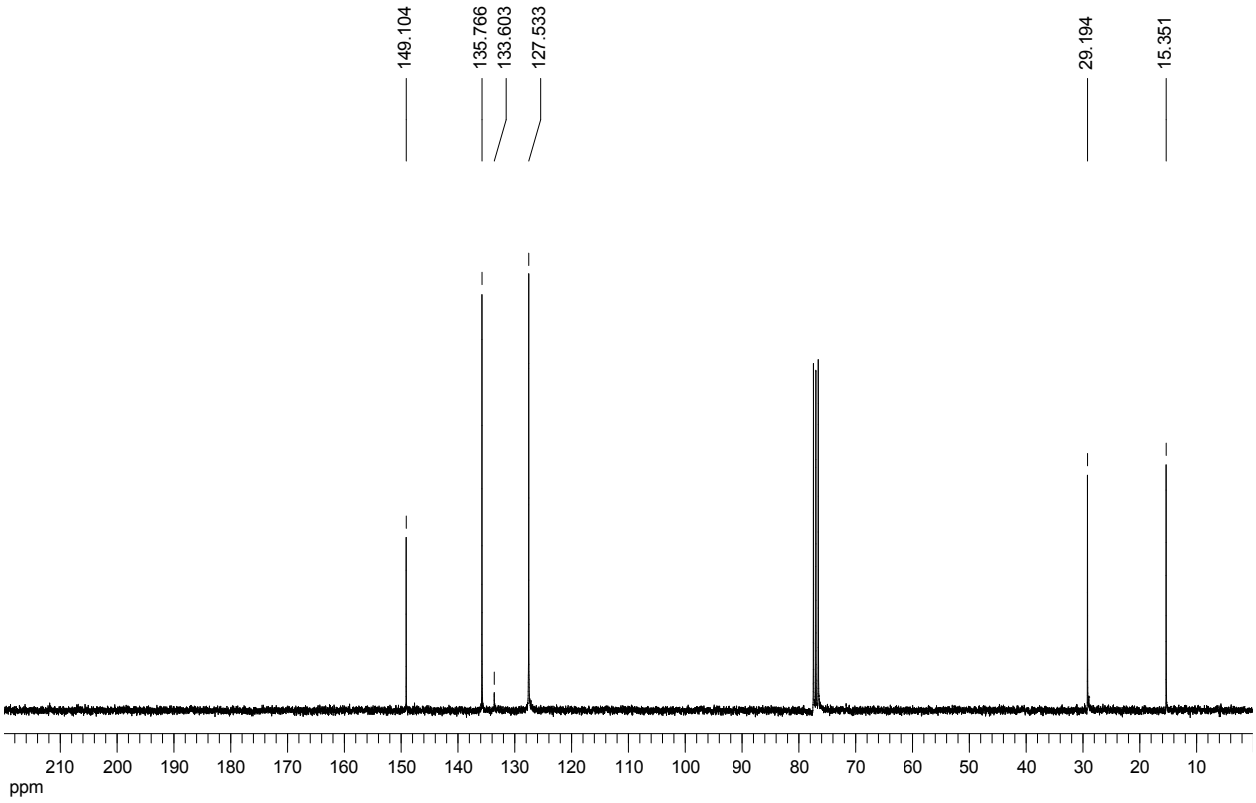
1,1'-Biphenyl]-4-yl(methyl)sulfane, 5k:

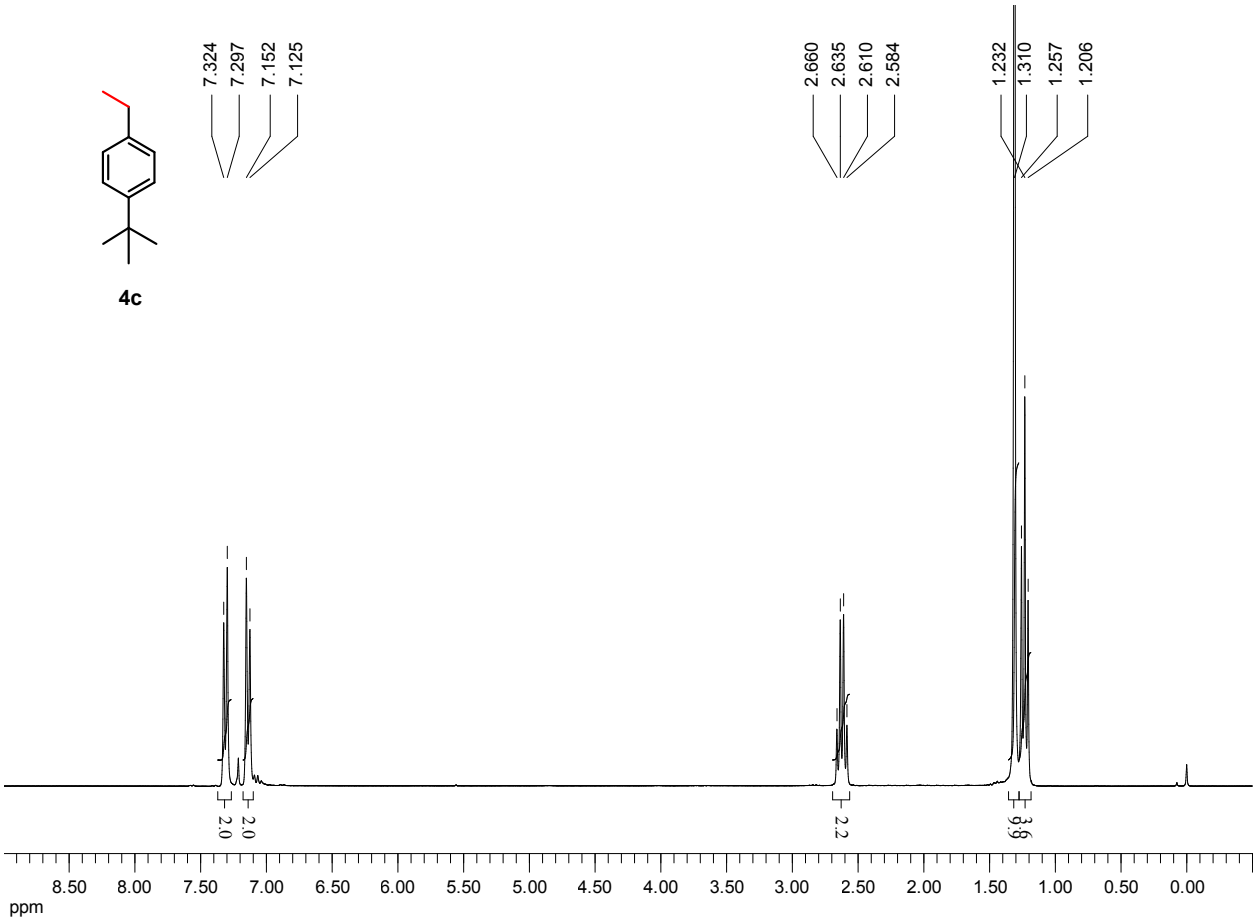


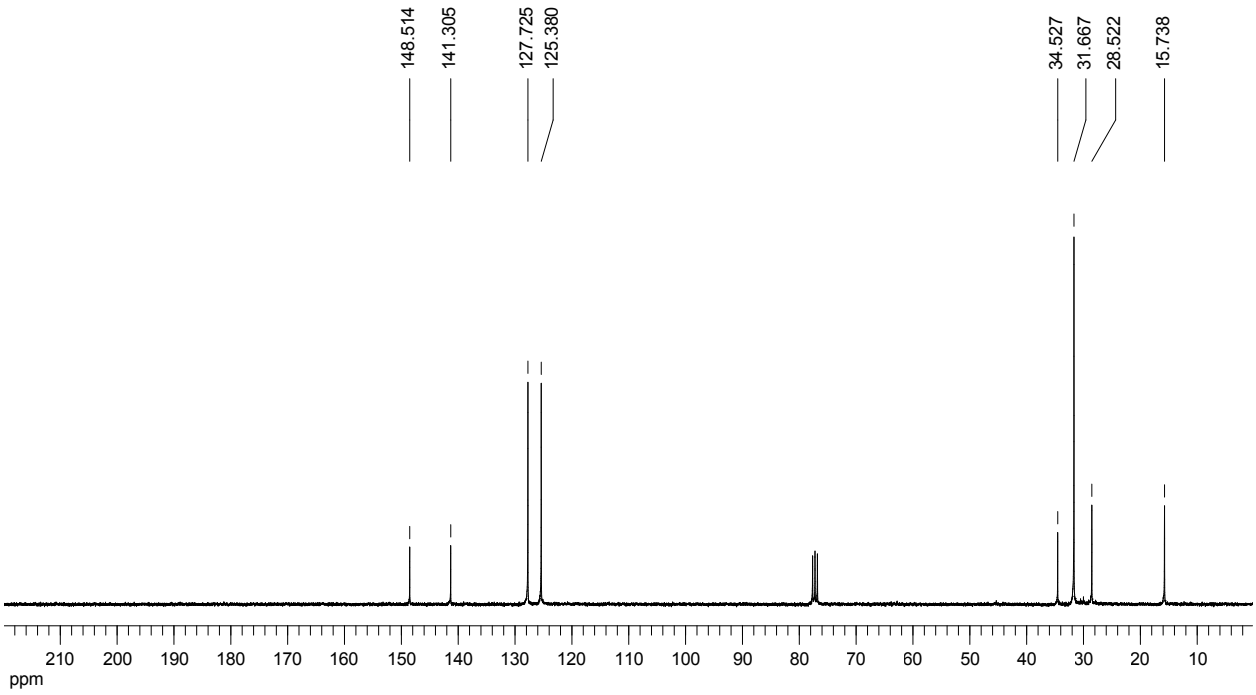
[161 mg, 96%, white solid]; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 7.49 (d, *J*=7.4 Hz, 2H), 7.41 (d, *J*=8.1 Hz, 2H), 7.33 (t, *J*=7.5 Hz, 2H), 7.24 (d, *J*=7.4 Hz, 1H), 7.16 (d, J=7.9 Hz, 2H; ^{13}C NMR (75 MHz, $CDCl_3$): δ= 141.2, 138.4, 137.1, 129.5, 128.7, 128.0, 127.1, 127.0, 21.1; IR ($CHCl_3$): 2956, 2924, 1729, 1488, 1459, 1441, 1215, 1009, 821, 666 cm^{-1}.

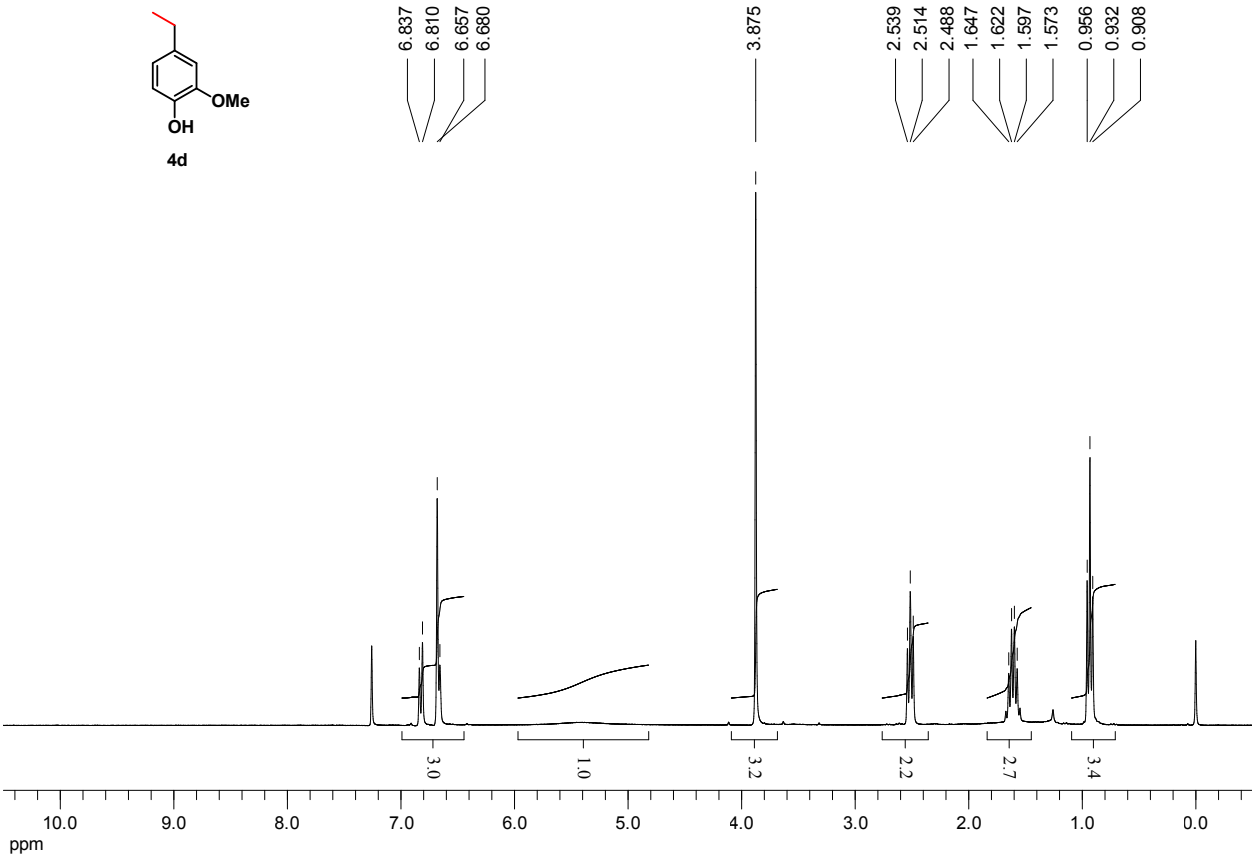

7.337
7.327
7.312
7.301
7.297
7.286
7.276
7.261
7.258
7.257
7.237
7.223
7.222
7.204
7.190
2.701
2.686
2.671
2.655
1.282
1.267
1.251
4a
4.98
2.13
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
144.145
128.189
127.744
125.464
28.761
15.518
175
163
150
138
125
113
100
88
75
63
50
38
25
13
0
ppm (t1)

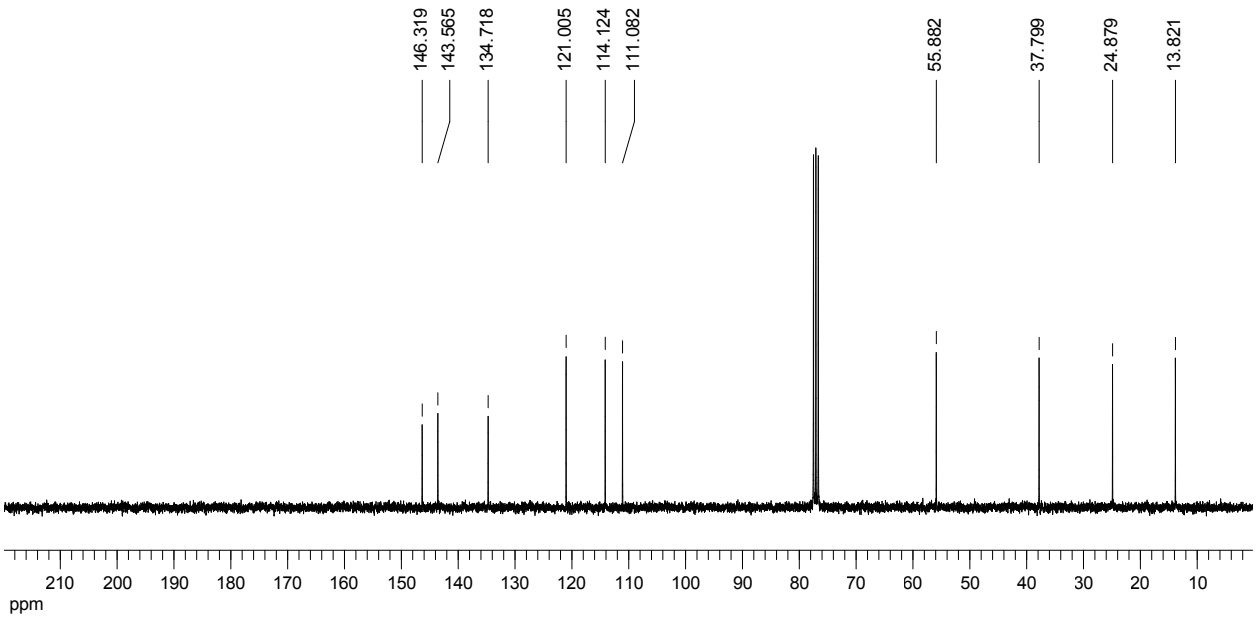

B(OH)2
4b
8.165
8.140
7.349
7.324
2.774
2.749
2.724
2.698
1.317
1.292
1.267
1.90
2.34
2.28
3.44
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

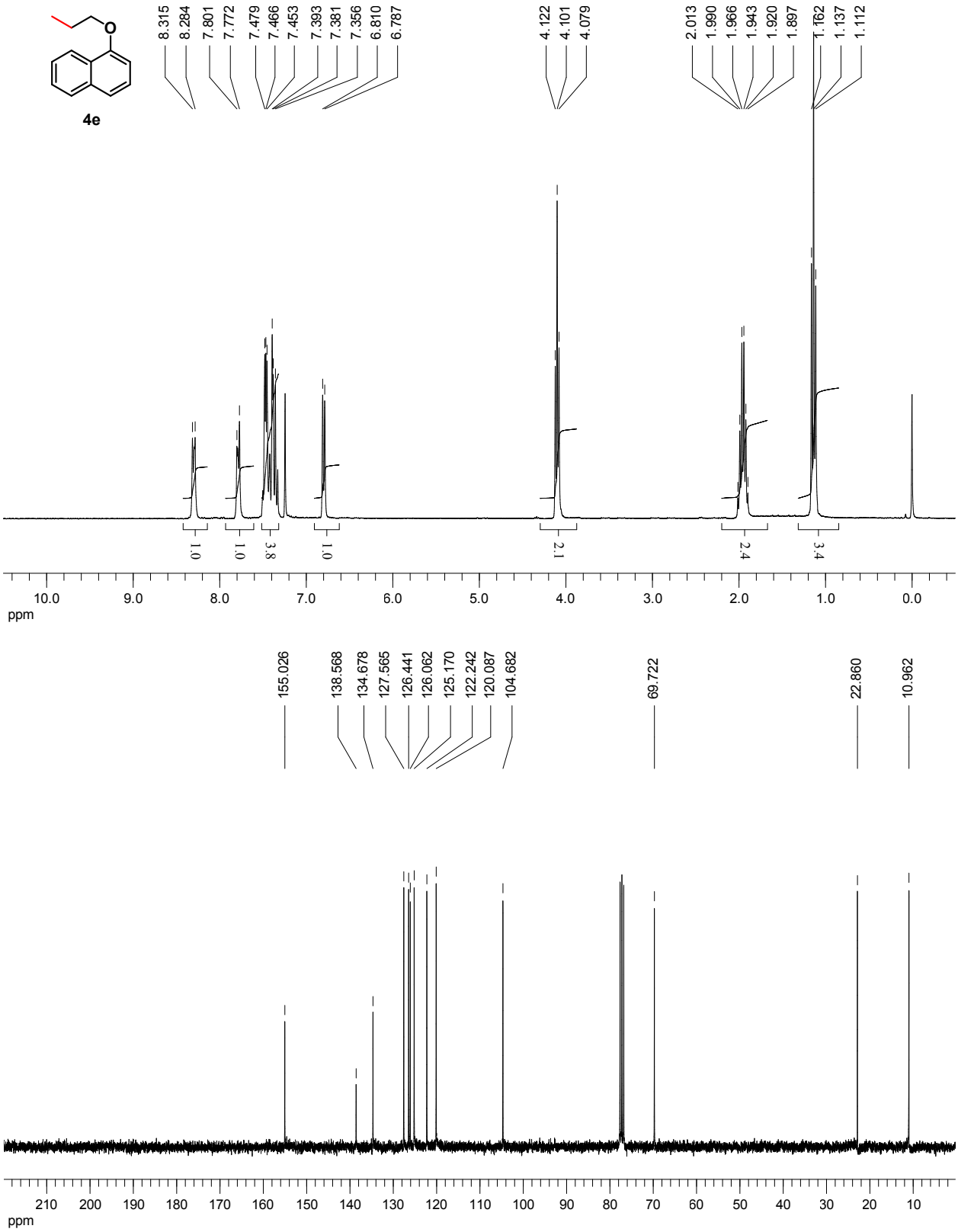

149.104
135.766
133.603
127.533
29.194
15.351
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

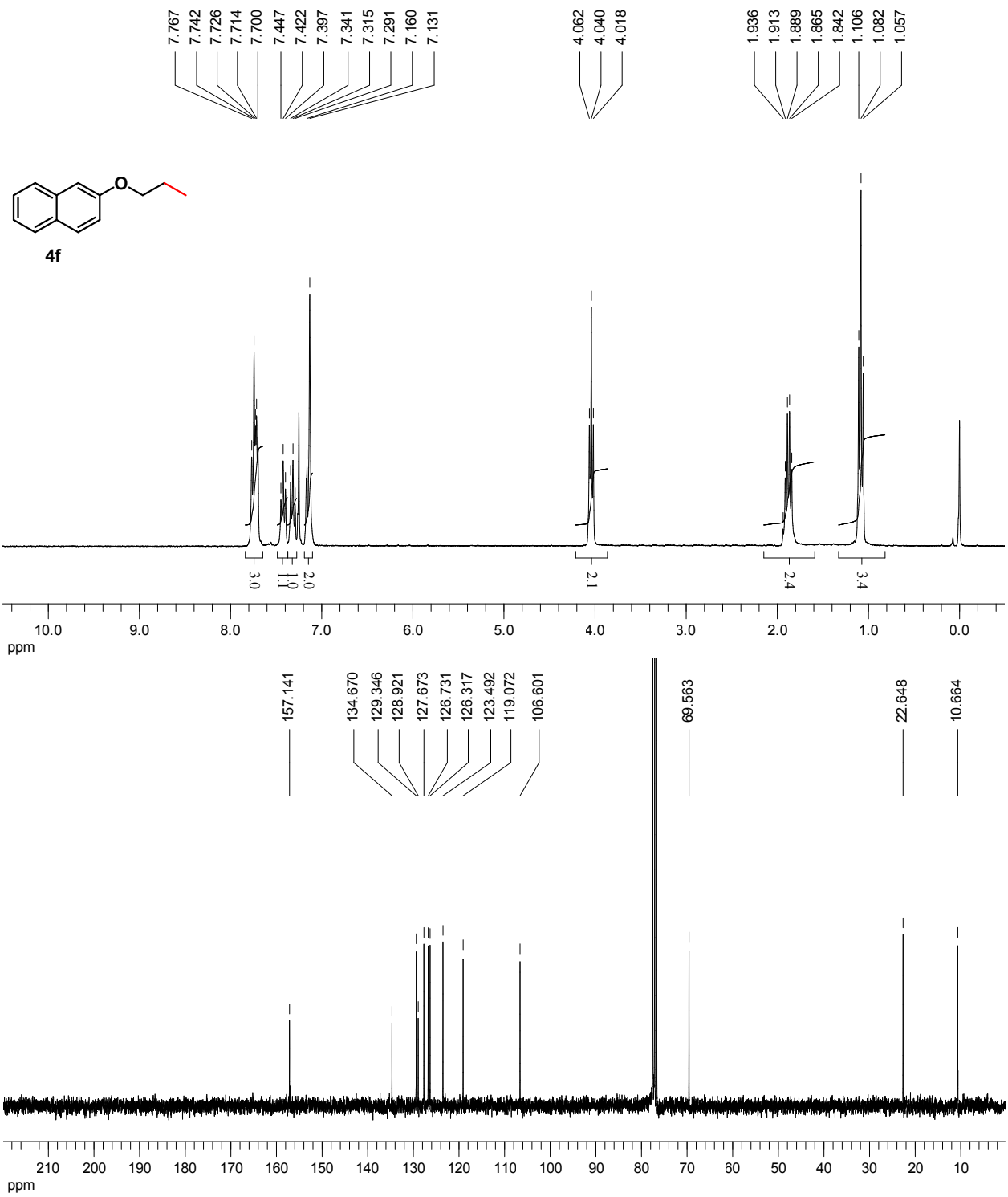

7.324
7.297
7.152
7.125
2.660
2.635
2.610
2.584
1.232
1.310
1.257
1.206
4c
2.0
2.0
2.2
9.6
8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm

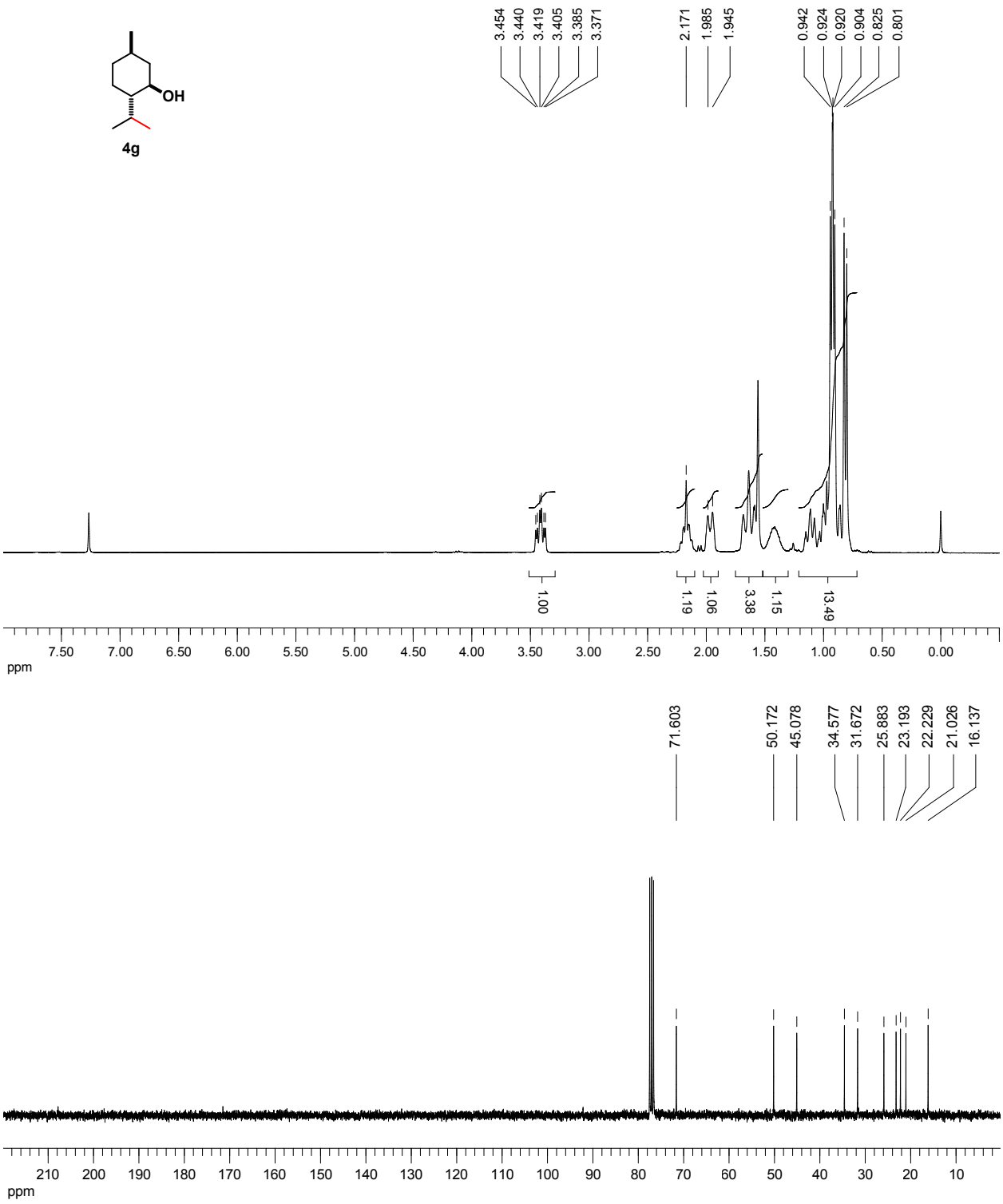

148.514
141.305
127.725
125.380
34.527
31.667
28.522
15.738
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

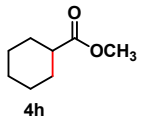

OMe
OH
4d
6.837
6.810
6.657
6.680
3.875
2.539
2.514
2.488
1.647
1.622
1.597
1.573
0.956
0.932
0.908
3.0
1.0
3.2
2.2
2.7
3.4
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


146.319
143.565
134.718
121.005
114.124
111.082
55.882
37.799
24.879
13.821
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


4e
8.315
8.284
7.801
7.772
7.479
7.466
7.453
7.393
7.381
7.356
6.810
6.787
4.122
4.101
4.079
2.013
1.990
1.966
1.943
1.920
1.897
1.162
1.137
1.112
1.0
1.0
3.8
1.0
2.1
2.4
3.4
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
155.026
138.568
134.678
127.565
126.441
126.062
125.170
122.242
120.087
104.682
69.722
22.860
10.962
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

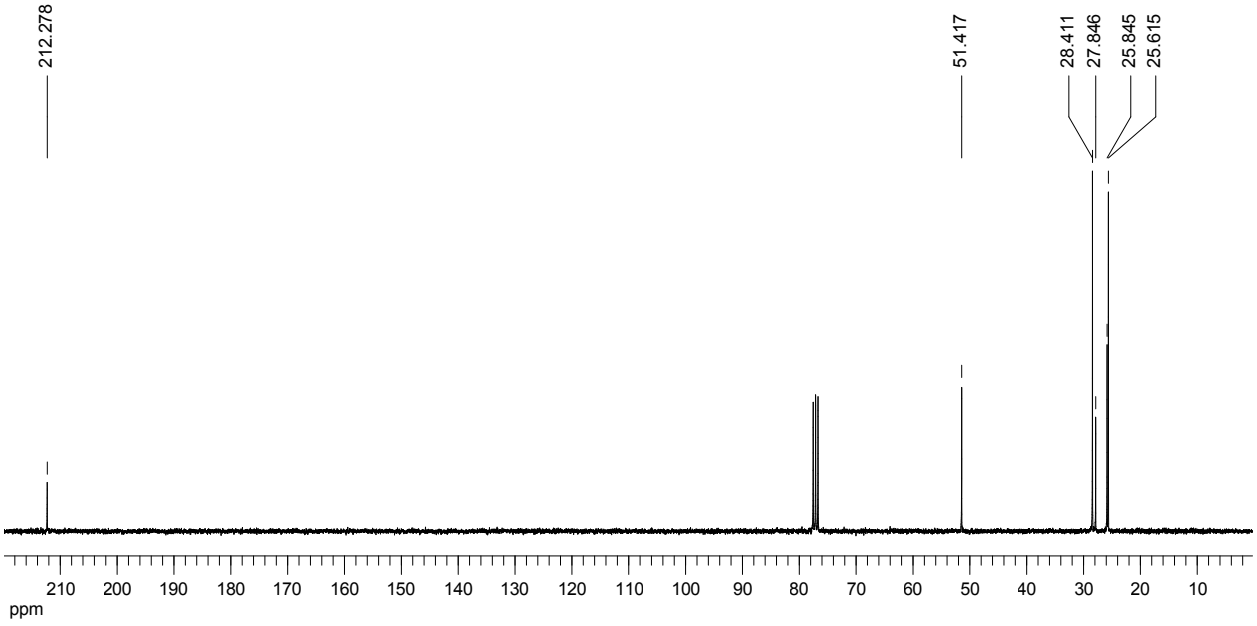

7.767
7.742
7.726
7.714
7.700
7.447
7.422
7.397
7.341
7.315
7.291
7.160
7.131
4.062
4.040
4.018
1.936
1.913
1.889
1.865
1.842
1.106
1.082
1.057
O
4f
3.0
1.1
1.0
2.0
2.1
2.4
3.4
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
157.141
134.670
129.346
128.921
127.673
126.731
126.317
123.492
119.072
106.601
69.563
22.648
10.664
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

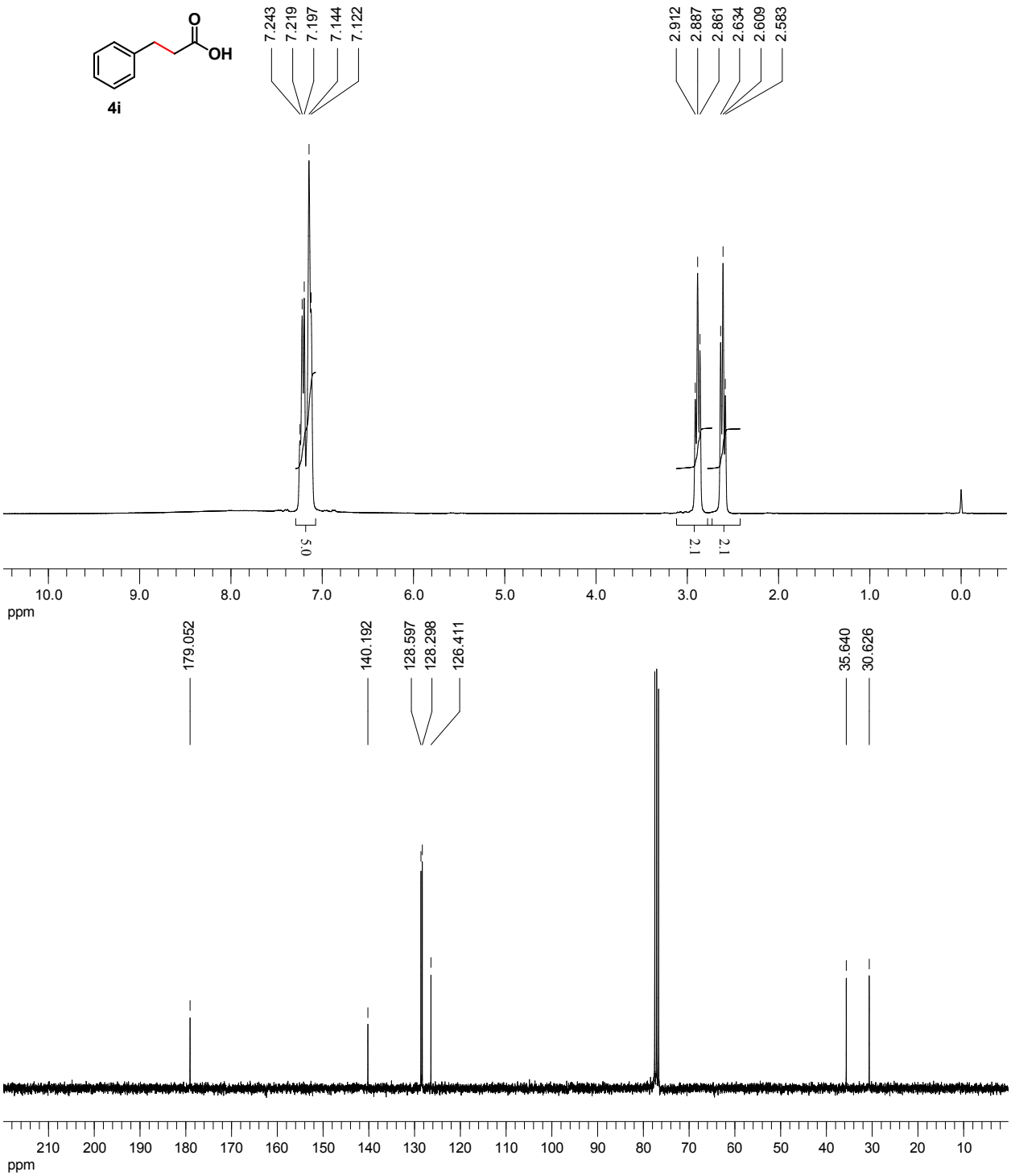

OH
4g
3.454
3.440
3.419
3.405
3.385
3.371
2.171
1.985
1.945
0.942
0.924
0.920
0.904
0.825
0.801
1.00
1.19
1.06
3.38
1.15
13.49
7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm
71.603
50.172
45.078
34.577
31.672
25.883
23.193
22.229
21.026
16.137
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

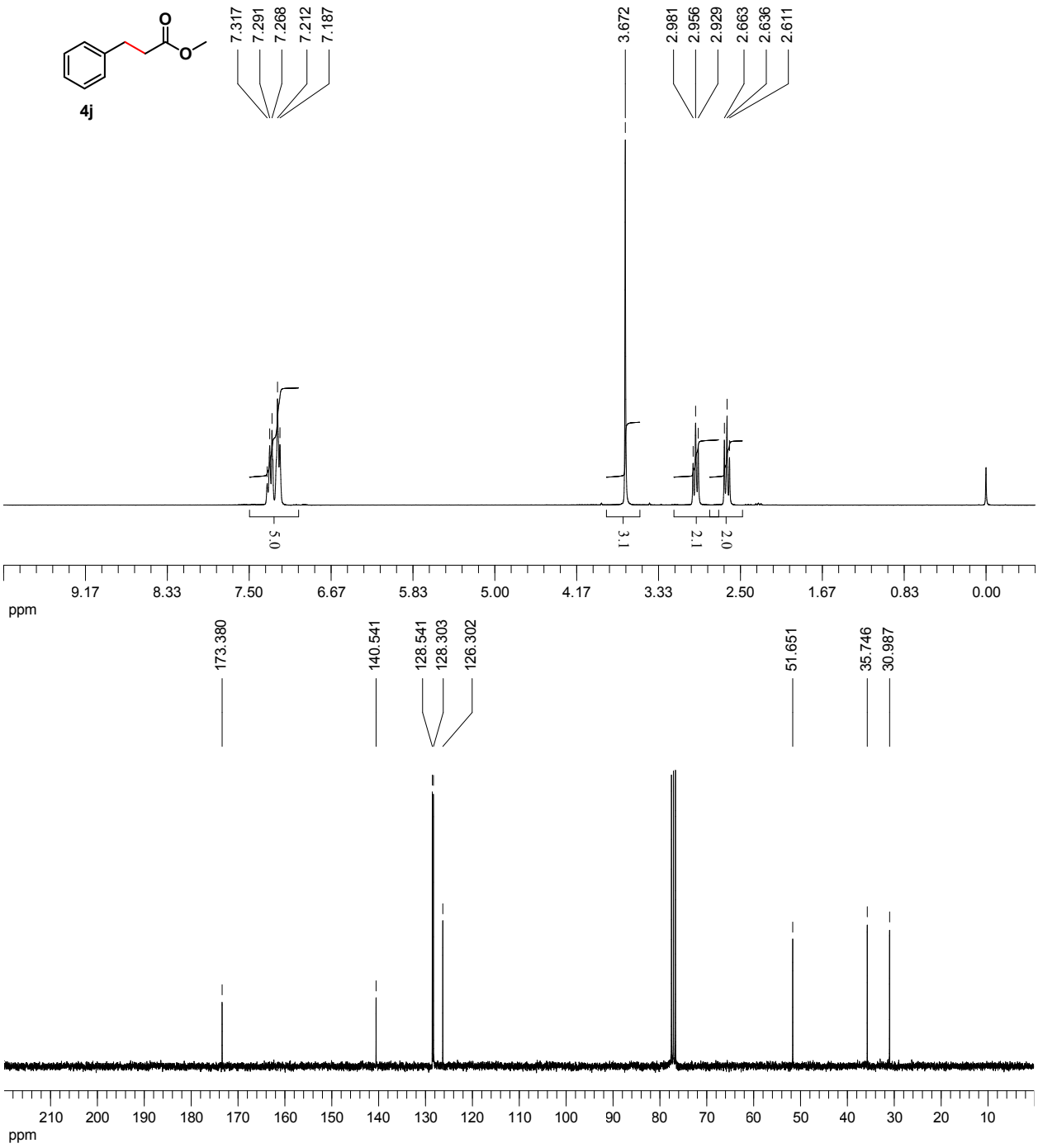

O
OCH3

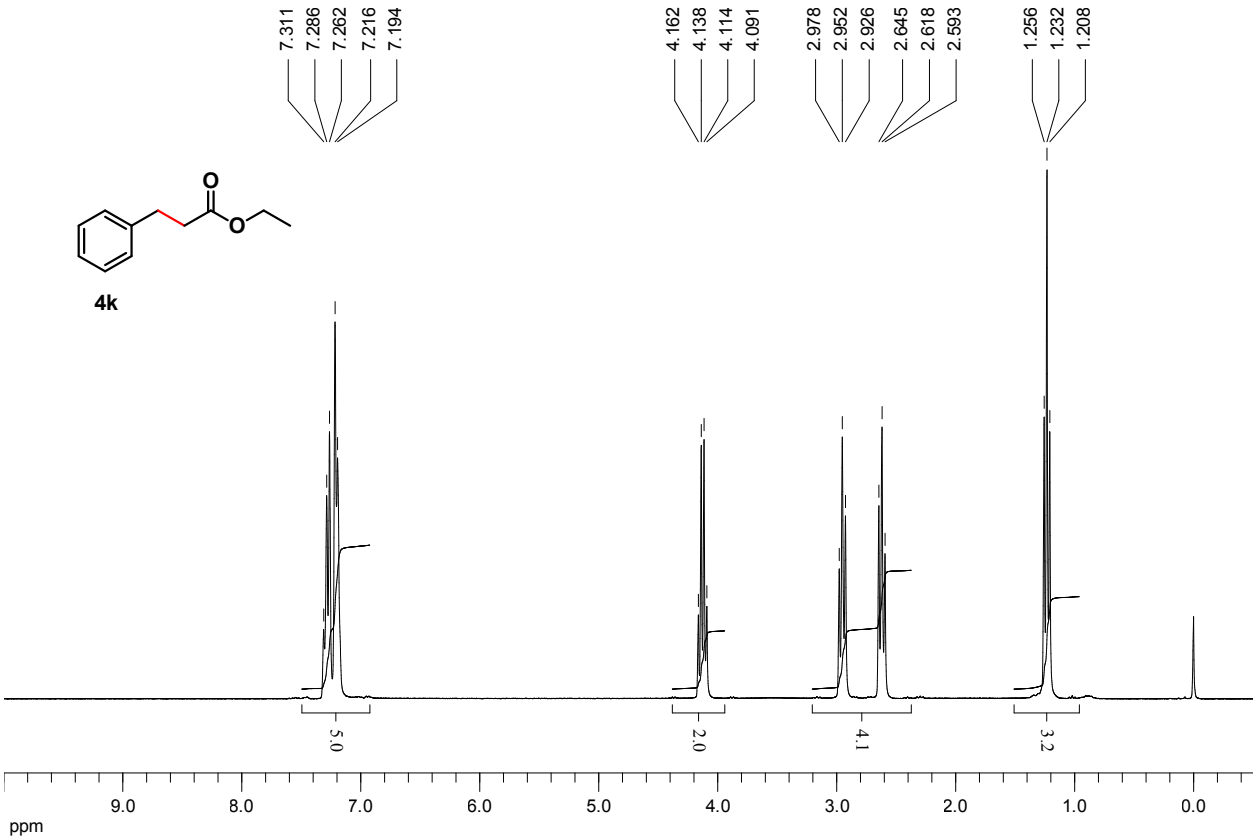
4h

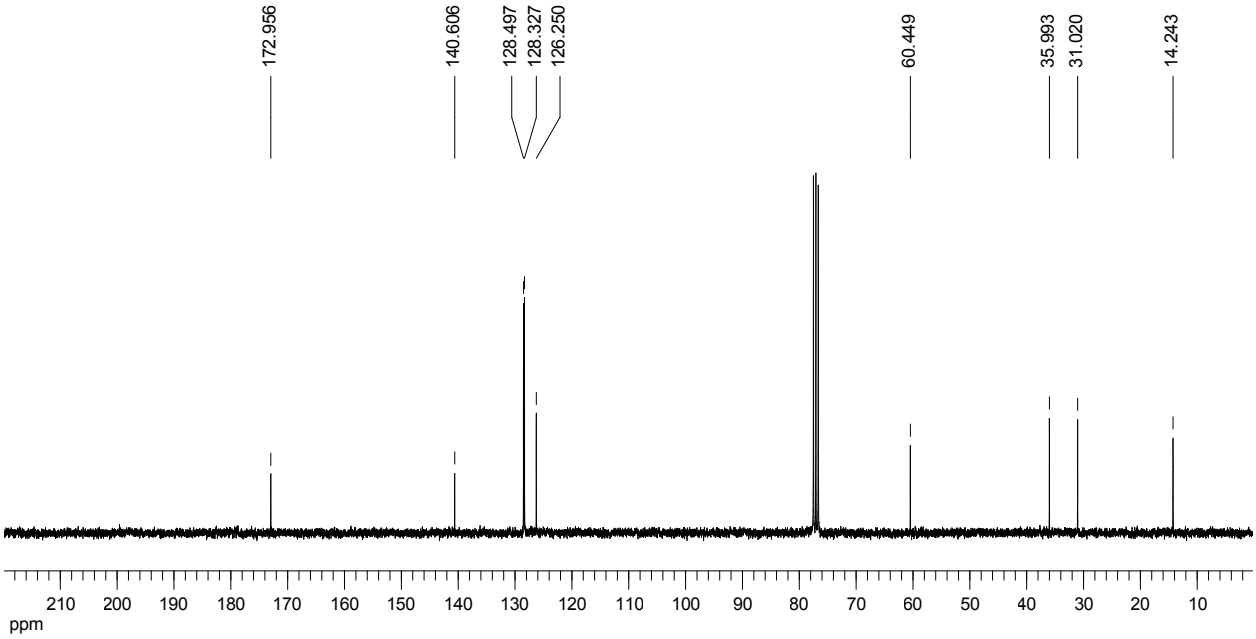
2.257
2.057
1.810
1.779
1.717
1.700
1.276
1.235
1.218
1.187
1.155
1.125
1.101
1.0
3.0
4.4
6.5
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
ppm

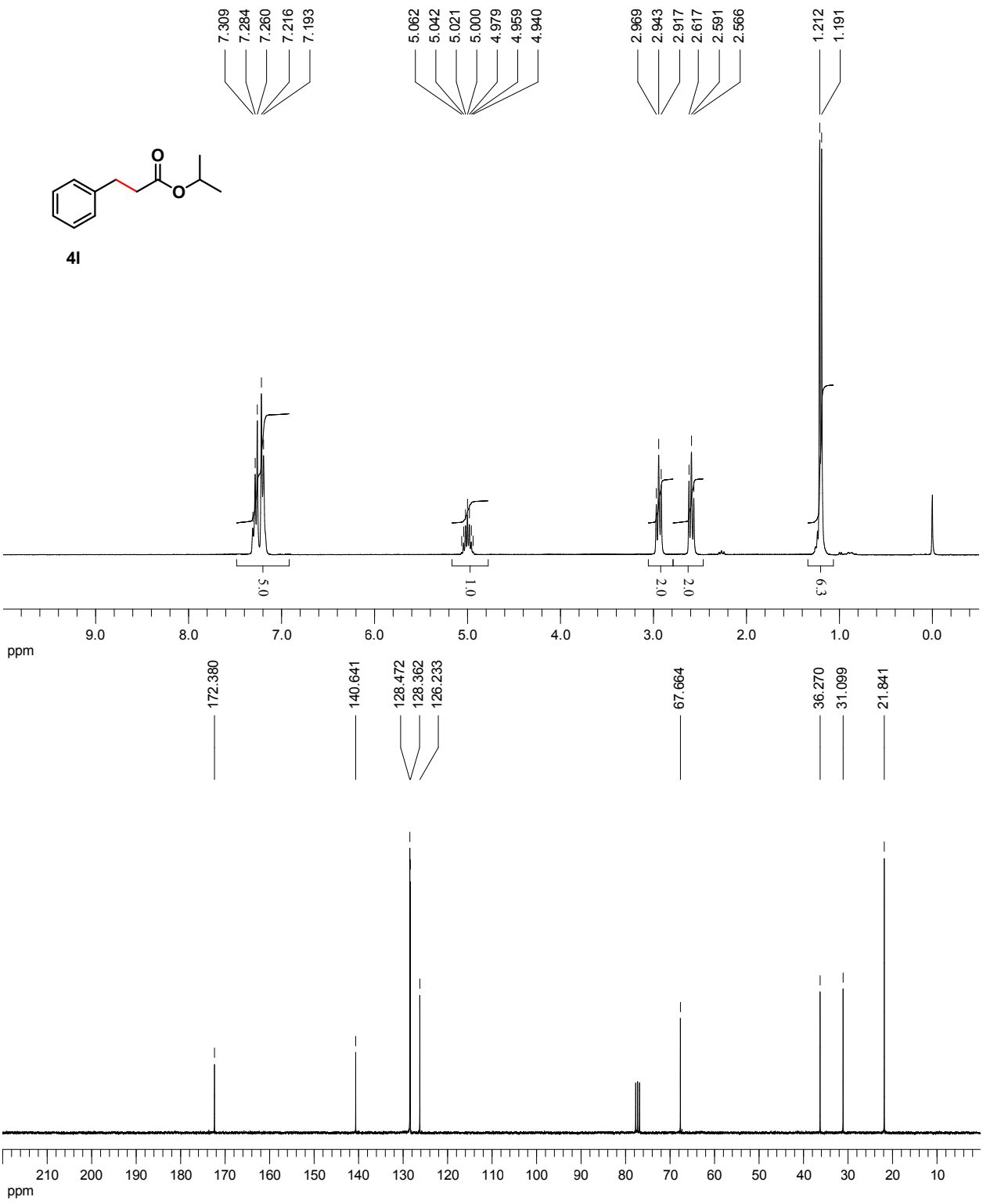

212.278
51.417
28.411
27.846
25.845
25.615
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

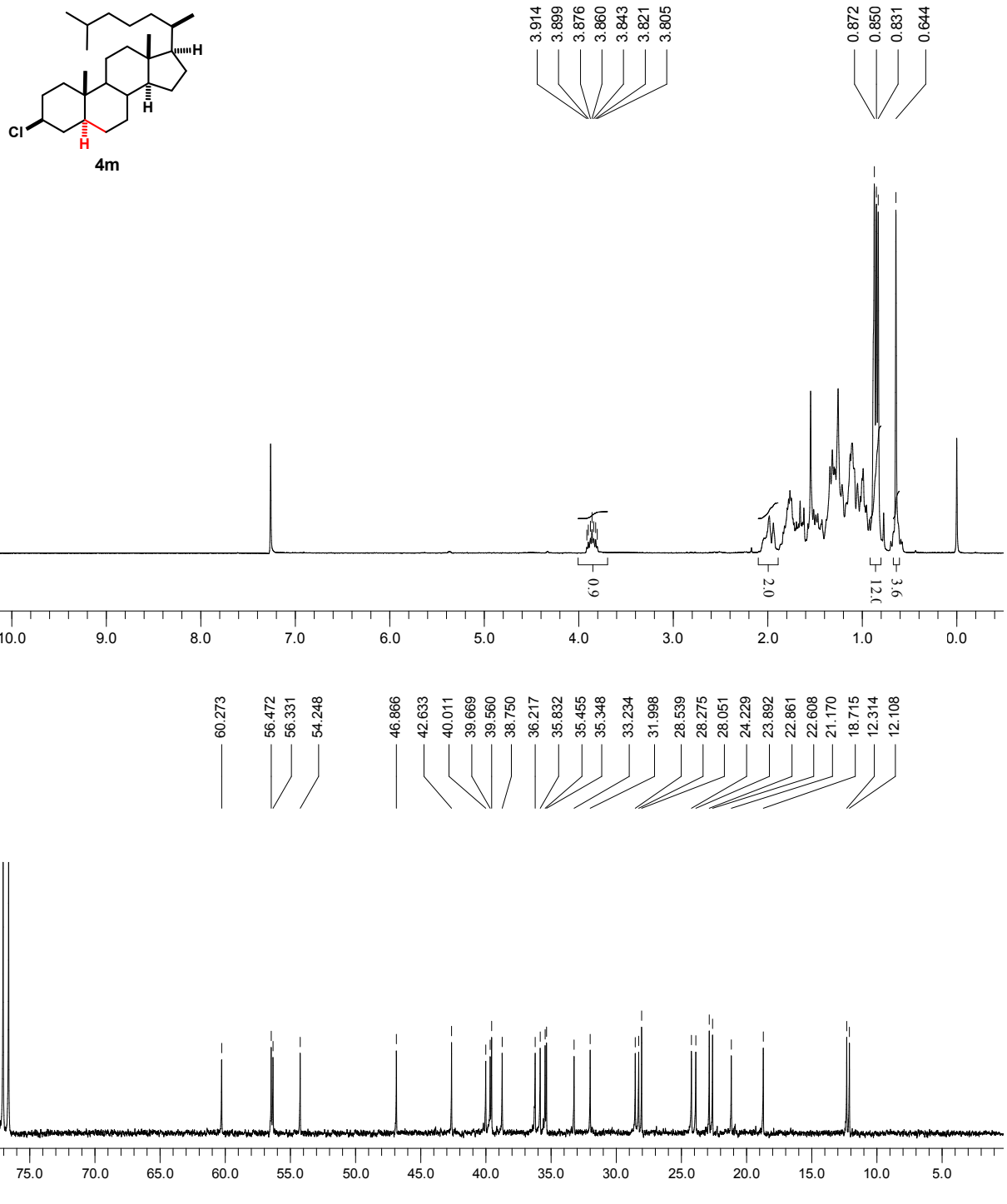

O
OH
4i
7.243
7.219
7.197
7.144
7.122
2.912
2.887
2.861
2.634
2.609
2.583
5.0
2.1
2.1
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
179.052
140.192
128.597
128.298
126.411
35.640
30.626
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

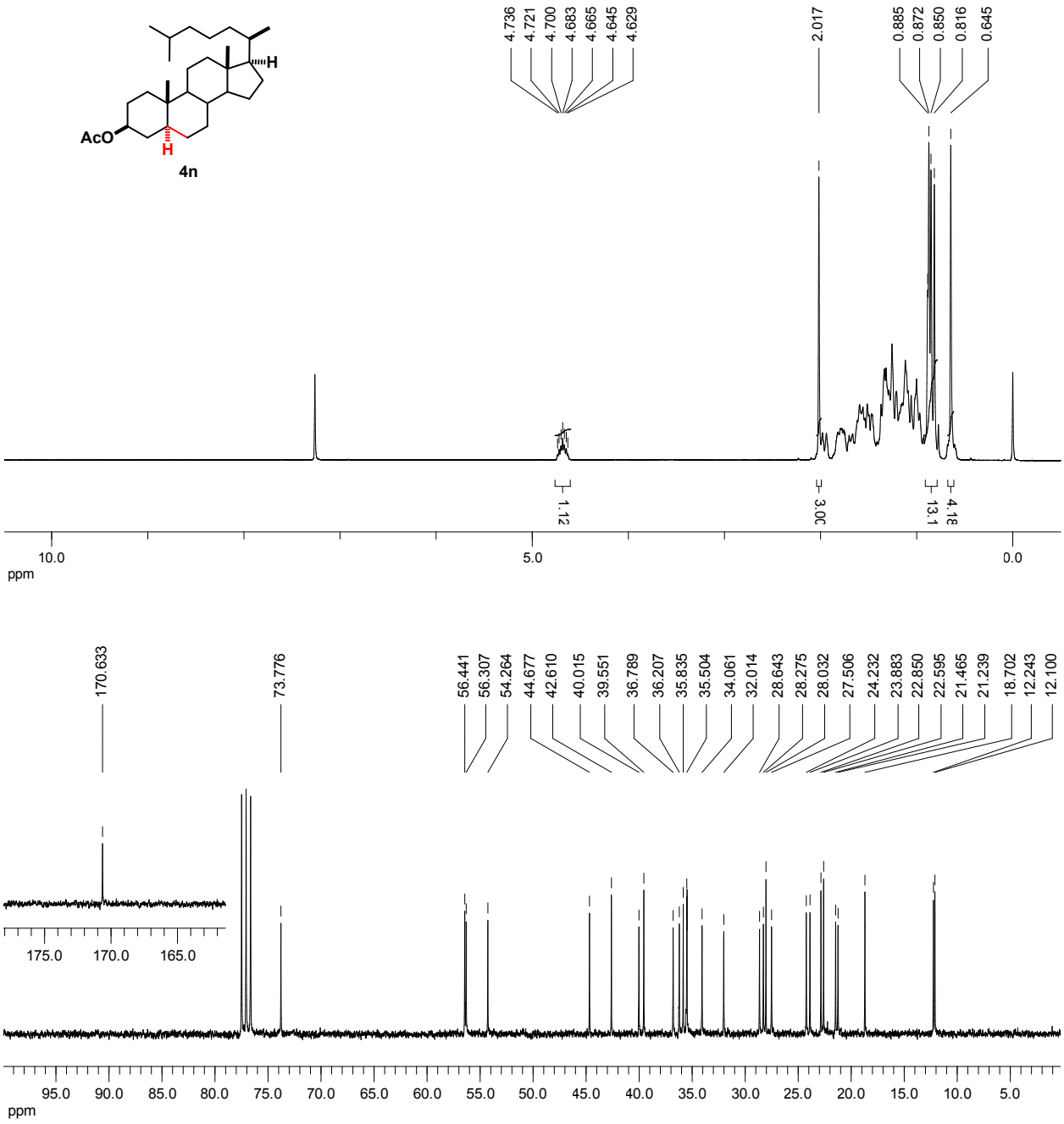

4j
7.317
7.291
7.268
7.212
7.187
3.672
2.981
2.956
2.929
2.663
2.636
2.611
5.0
3.1
2.1
2.0
9.17
8.33
7.50
6.67
5.83
5.00
4.17
3.33
2.50
1.67
0.83
0.00
ppm
173.380
140.541
128.541
128.303
126.302
51.651
35.746
30.987
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.311
7.286
7.262
7.216
7.194
4.162
4.138
4.114
4.091
2.978
2.952
2.926
2.645
2.618
2.593
1.256
1.232
1.208
O
O
4k
5.0
2.0
4.1
3.2
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


172.956
140.606
128.497
128.327
126.250
60.449
35.993
31.020
14.243
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.309
7.284
7.260
7.216
7.193
5.062
5.042
5.021
5.000
4.979
4.959
4.940
2.969
2.943
2.917
2.617
2.591
2.566
1.212
1.191
O
O
4l
5.0
1.0
2.0
2.0
6.3
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
172.380
140.641
128.472
128.362
126.233
67.664
36.270
31.099
21.841
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
H
H
H
4m
3.914
3.899
3.876
3.860
3.843
3.821
3.805
0.872
0.850
0.831
0.644
0.9
2.0
12.1
3.6
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm
60.273
56.472
56.331
54.248
46.866
42.633
40.011
39.669
39.560
38.750
36.217
35.832
35.455
35.348
33.234
31.998
28.539
28.275
28.051
24.229
23.892
22.861
22.608
21.170
18.715
12.314
12.108
75.0
70.0
65.0
60.0
55.0
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
ppm


AcO
H
H
4n
4.736
4.721
4.700
4.683
4.665
4.645
4.629
2.017
0.885
0.872
0.850
0.816
0.645
1.12
3.00
13.1
4.18
10.0
5.0
0.0
ppm
170.633
73.776
56.441
56.307
54.264
44.677
42.610
40.015
39.551
36.789
36.207
35.835
35.504
34.061
32.014
28.643
28.275
28.032
27.506
24.232
23.883
22.850
22.595
21.465
21.239
18.702
12.243
12.100
175.0
170.0
165.0
95.0
90.0
85.0
80.0
75.0
70.0
65.0
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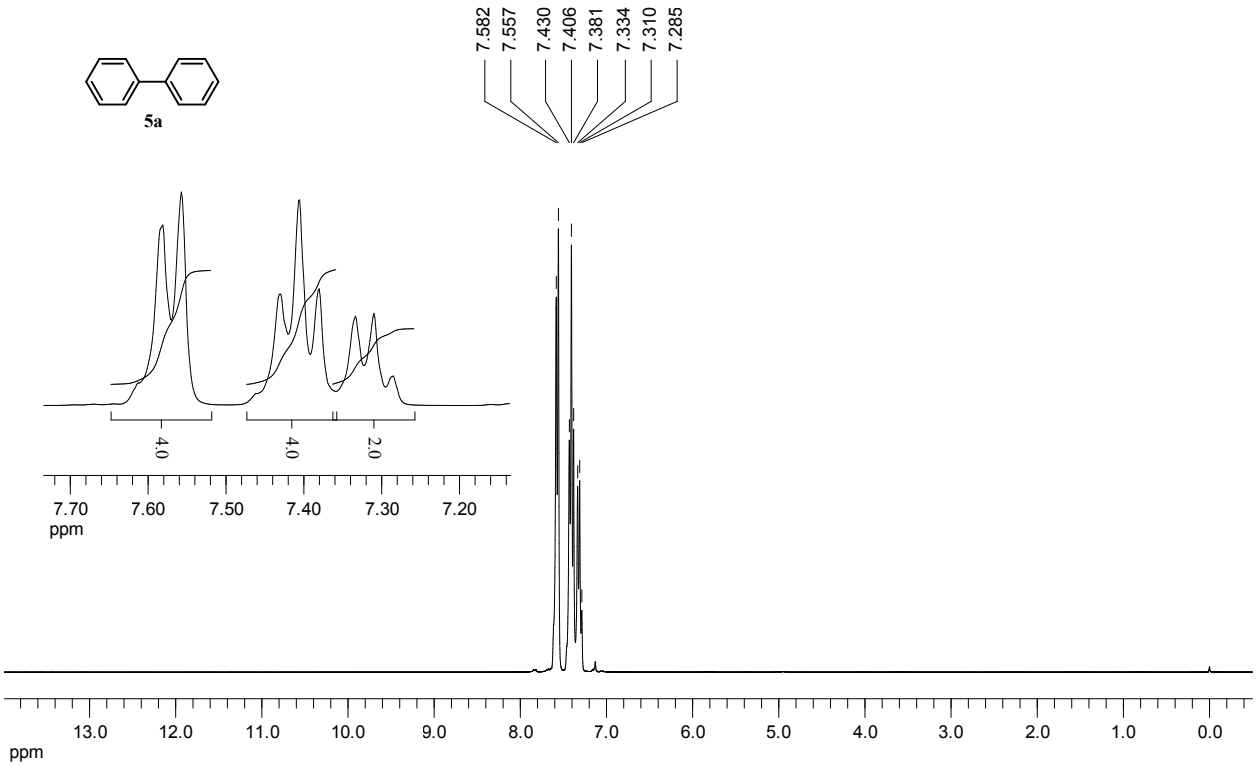
7.582
7.557
7.430
7.406
7.381
7.334
7.310
7.285
5a
4.0
4.0
2.0
7.70
7.60
7.50
7.40
7.30
7.20
ppm
13.0
12.0
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8.0
7.0
6.0
5.0
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3.0
2.0
1.0
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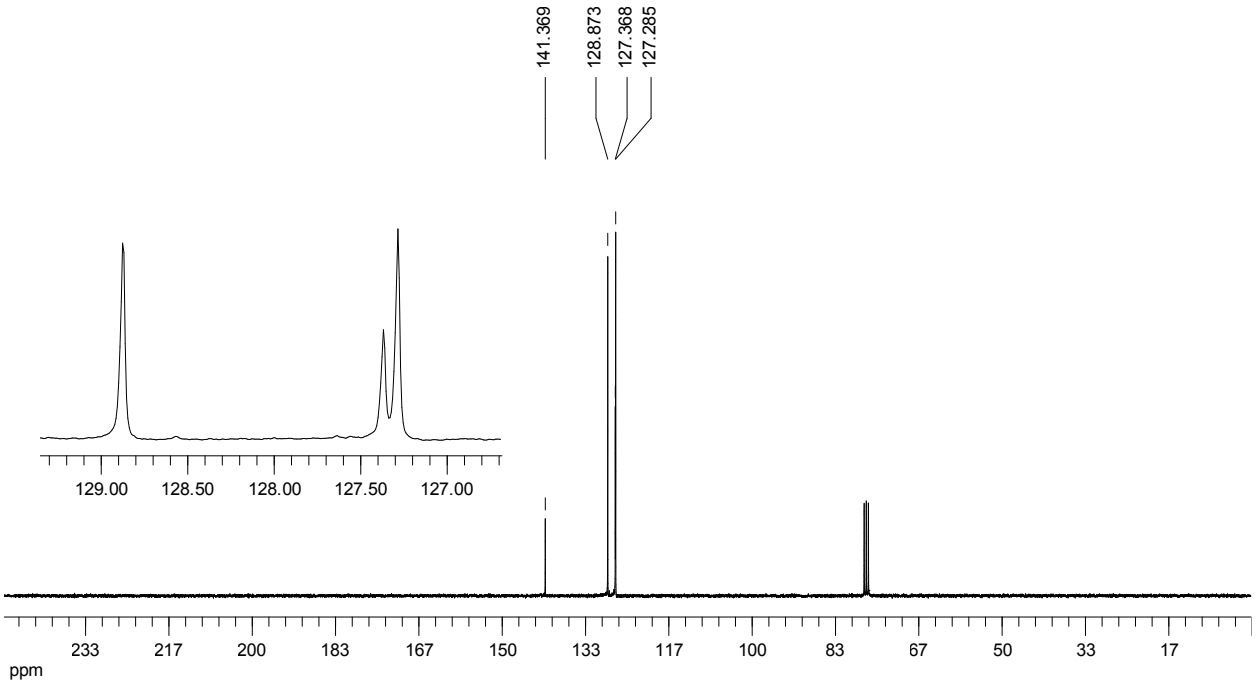
141.369
128.873
127.368
127.285
129.00
128.50
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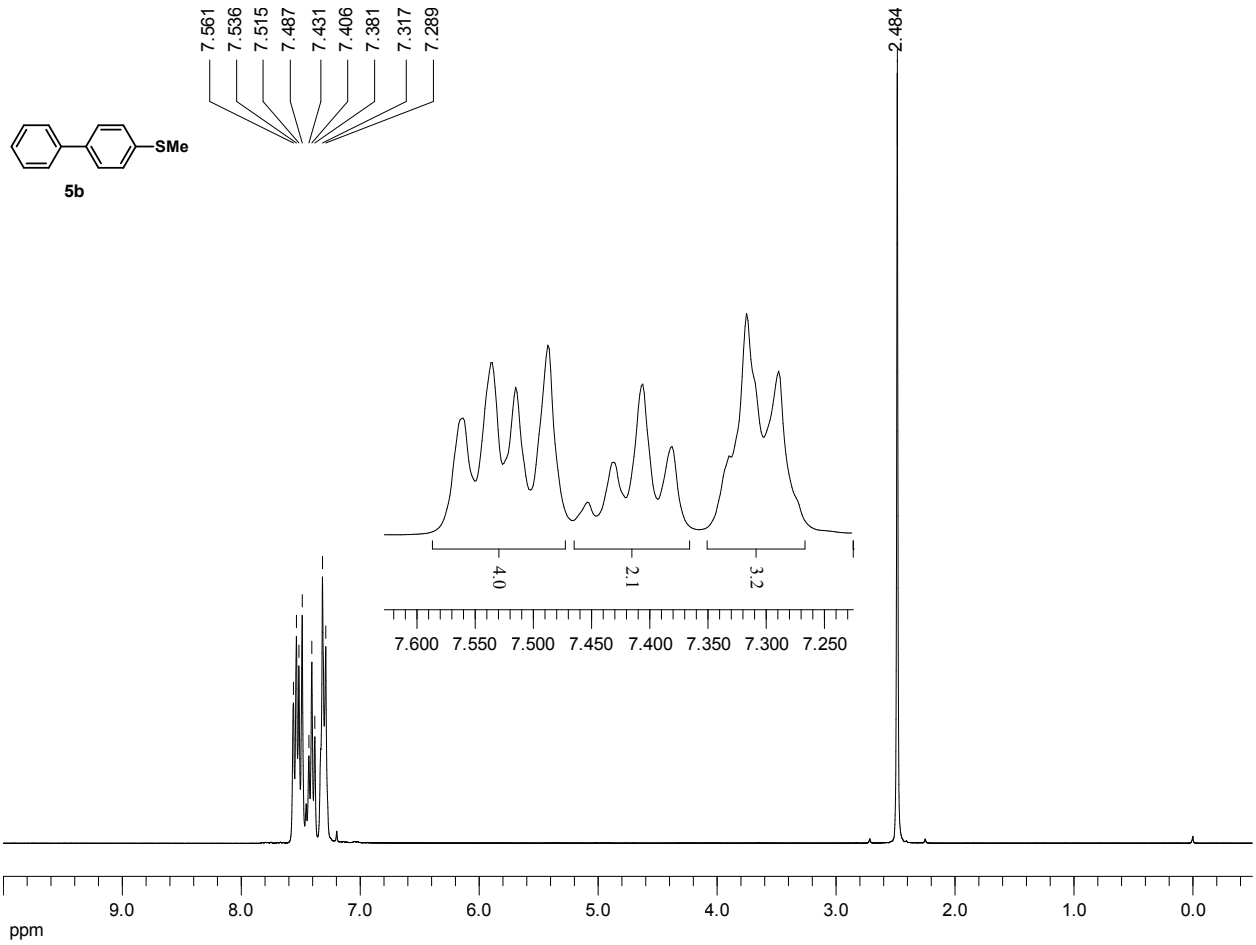
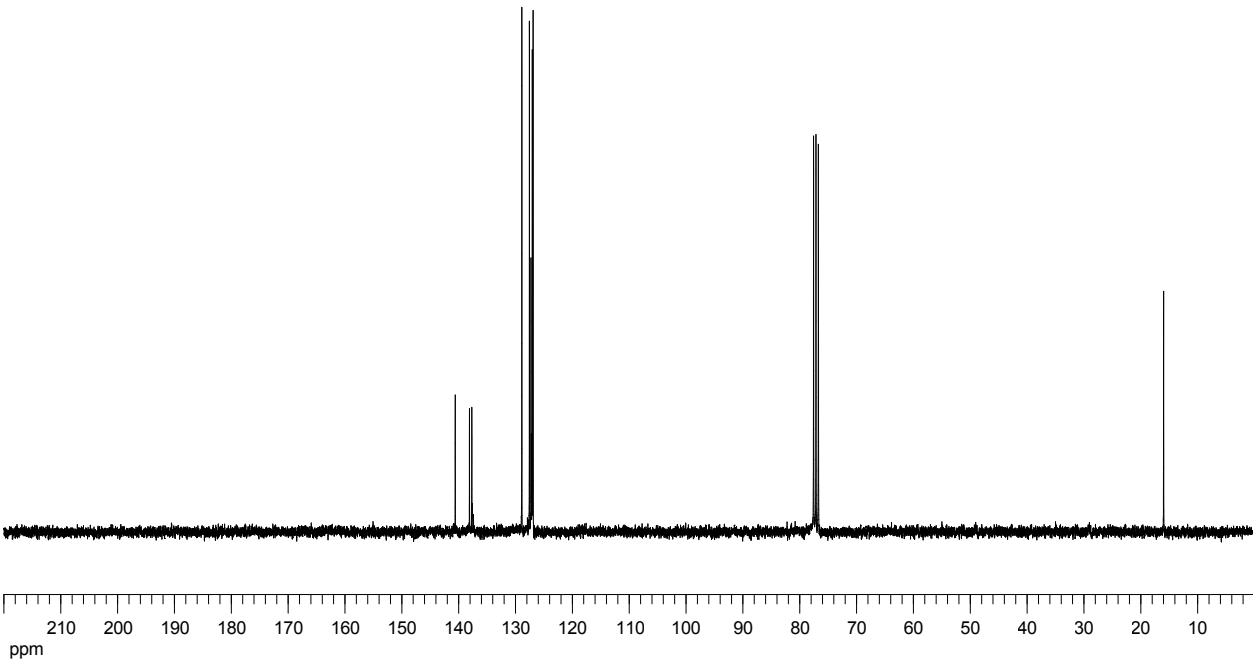
127.00
233
217
200
183
167
150
133
117
100
83
67
50
33
17
ppm


7.561
7.536
7.515
7.487
7.431
7.406
7.381
7.317
7.289
2.484
SMe
5b
4.0
2.1
3.2
7.600 7.550 7.500 7.450 7.400 7.350 7.300 7.250
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm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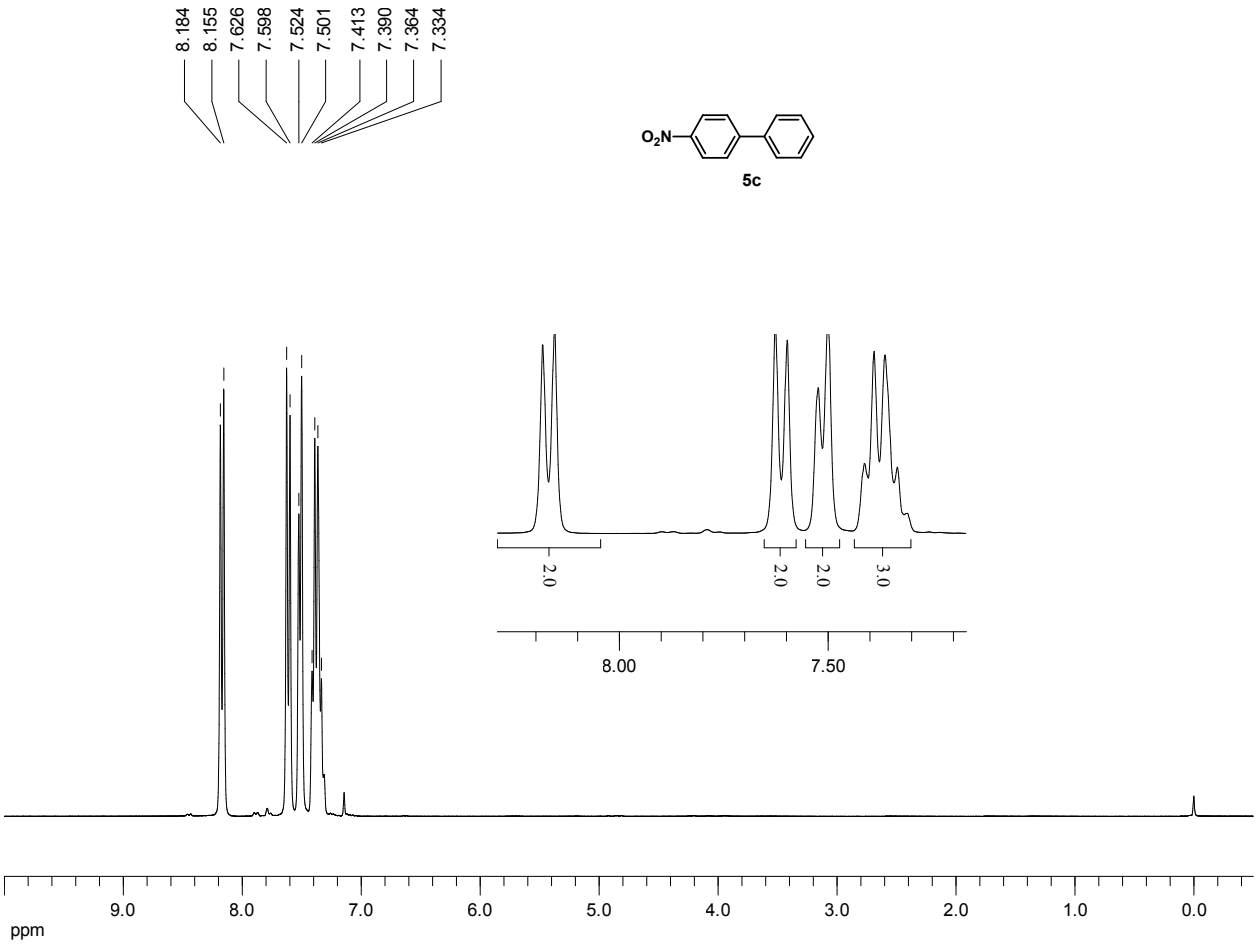
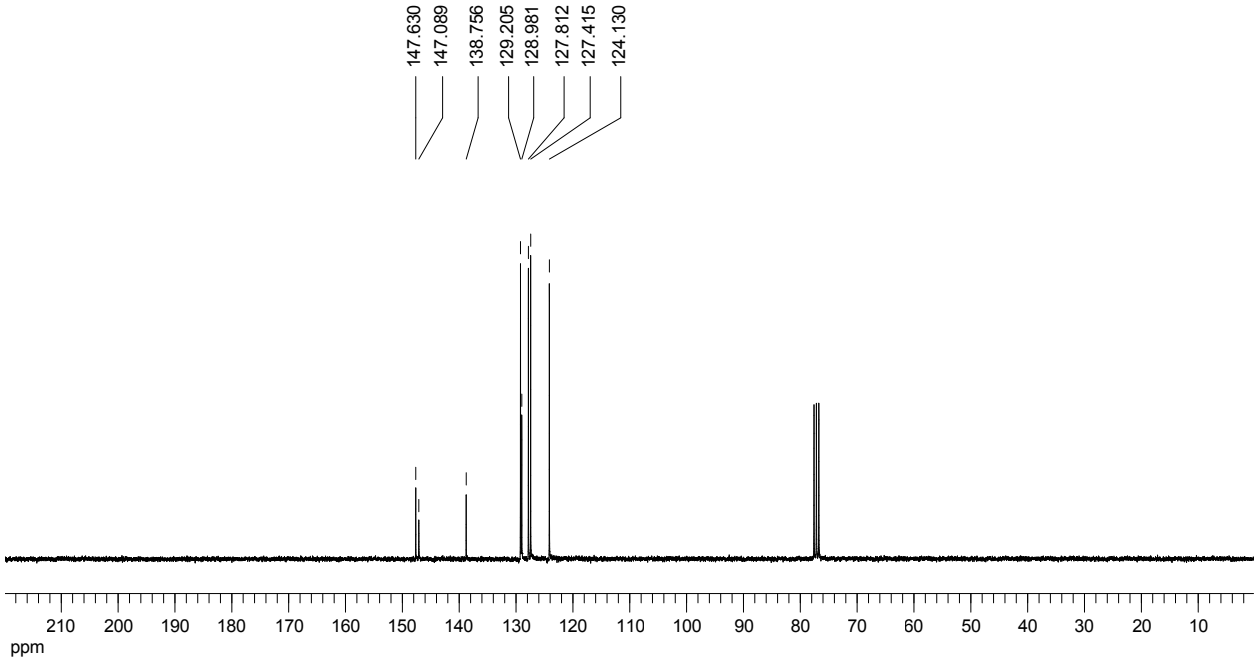
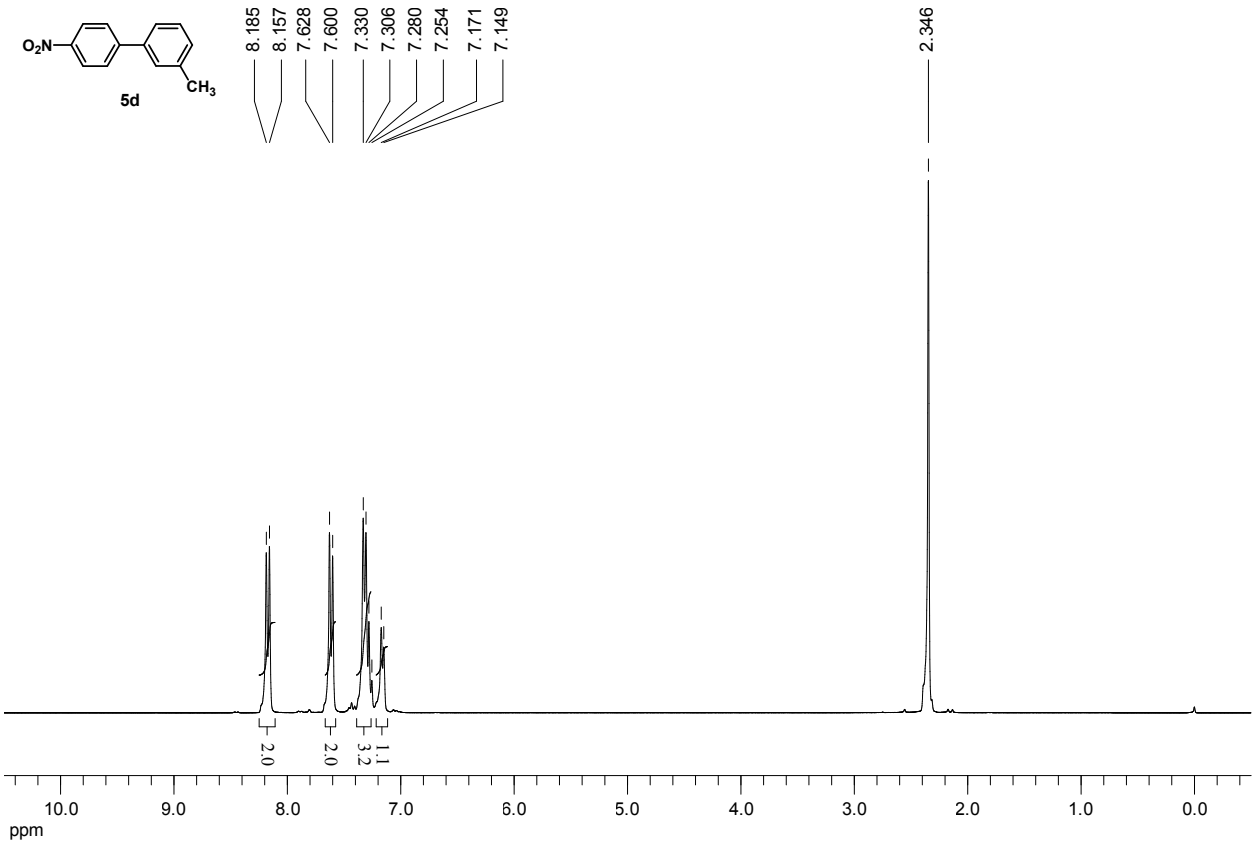
ppm


8.184
8.155
7.626
7.598
7.524
7.501
7.413
7.390
7.364
7.334
O2N
5c
2.0
2.0
2.0
3.0
8.00
7.50
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


147.630
147.089
138.756
129.205
128.981
127.812
127.415
124.130
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O2N
CH3
5d
8.185
8.157
7.628
7.600
7.330
7.306
7.280
7.254
7.171
7.149
2.346
2.0
2.0
3.2
1.1
10.0
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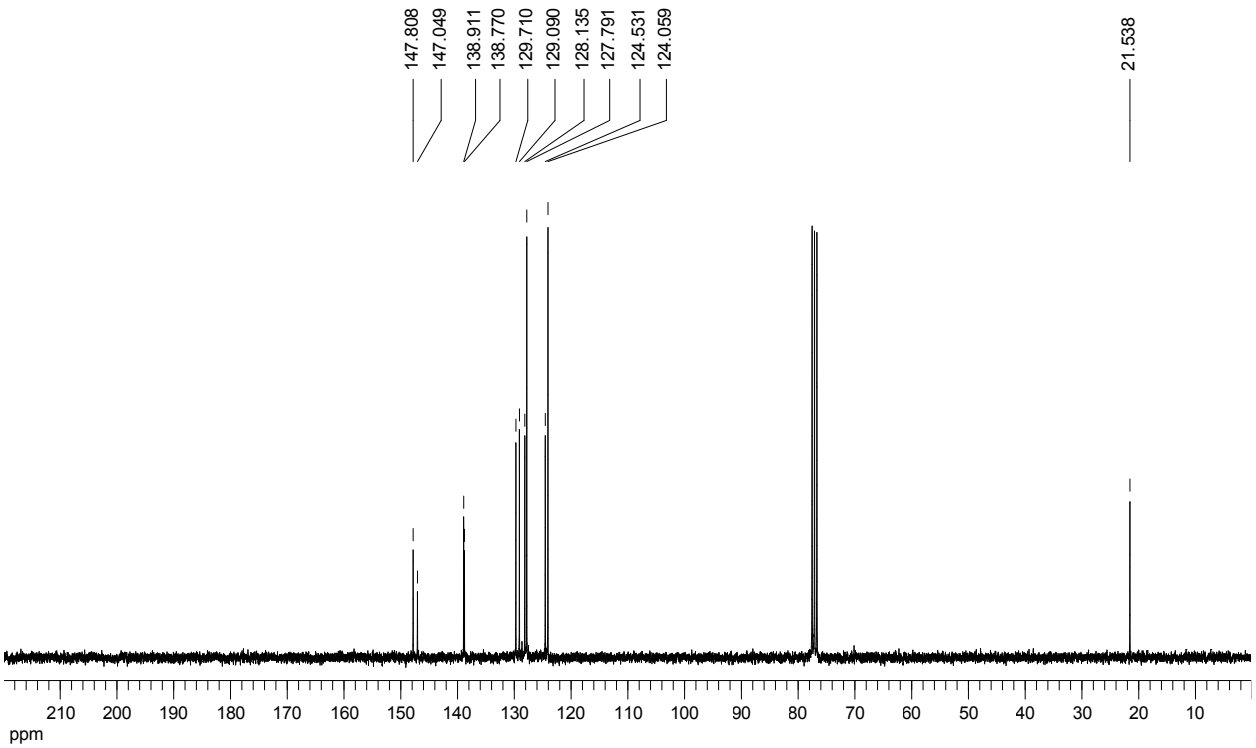
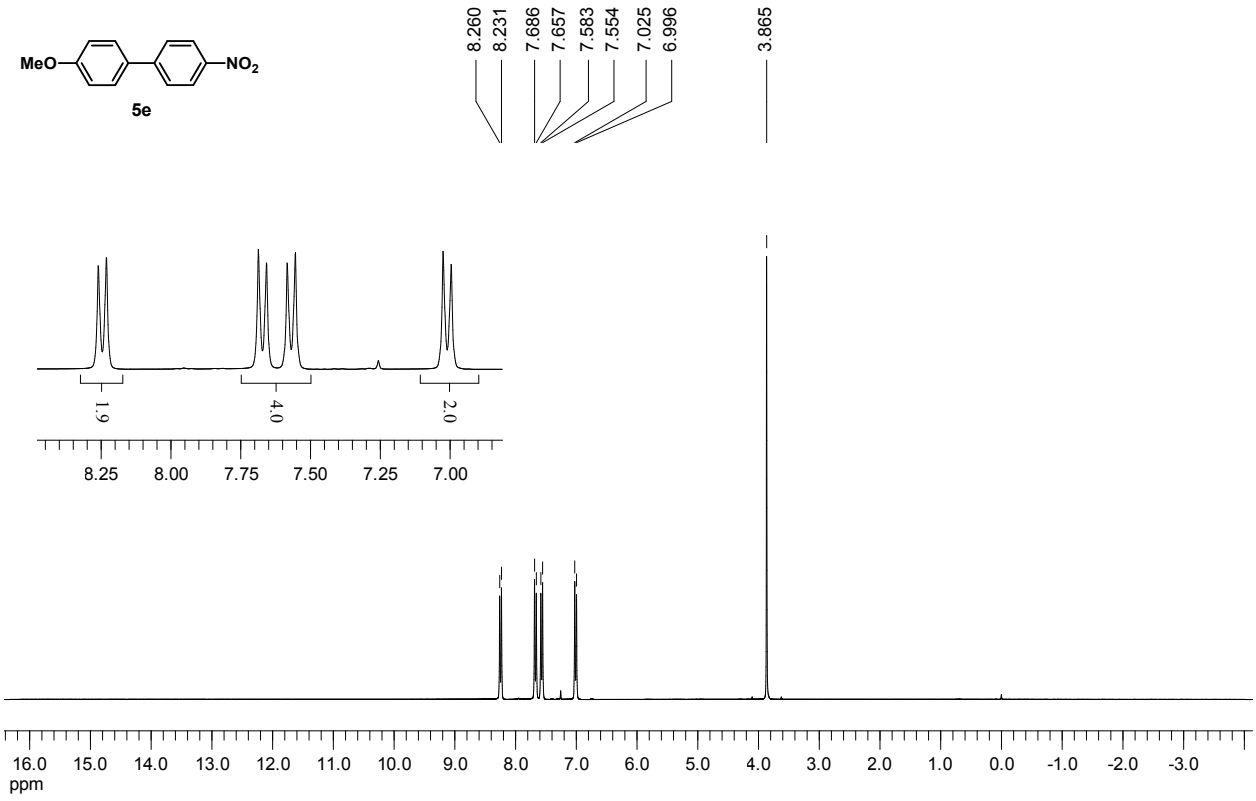
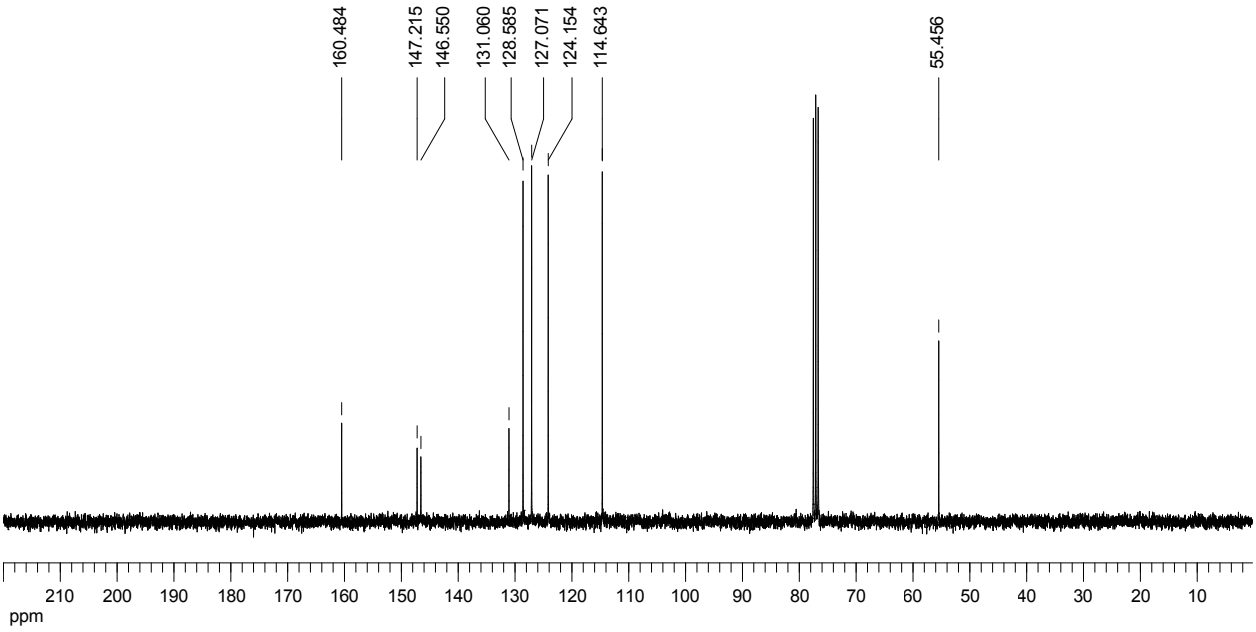
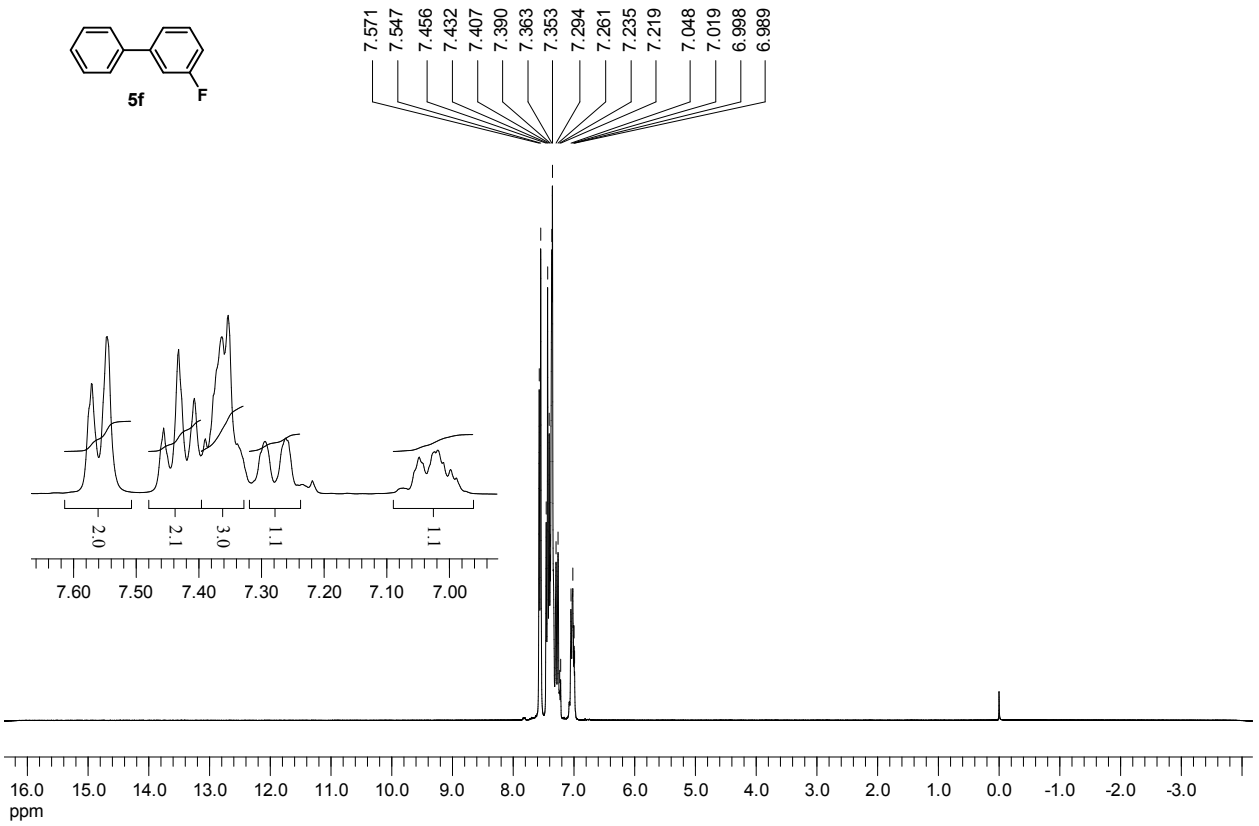
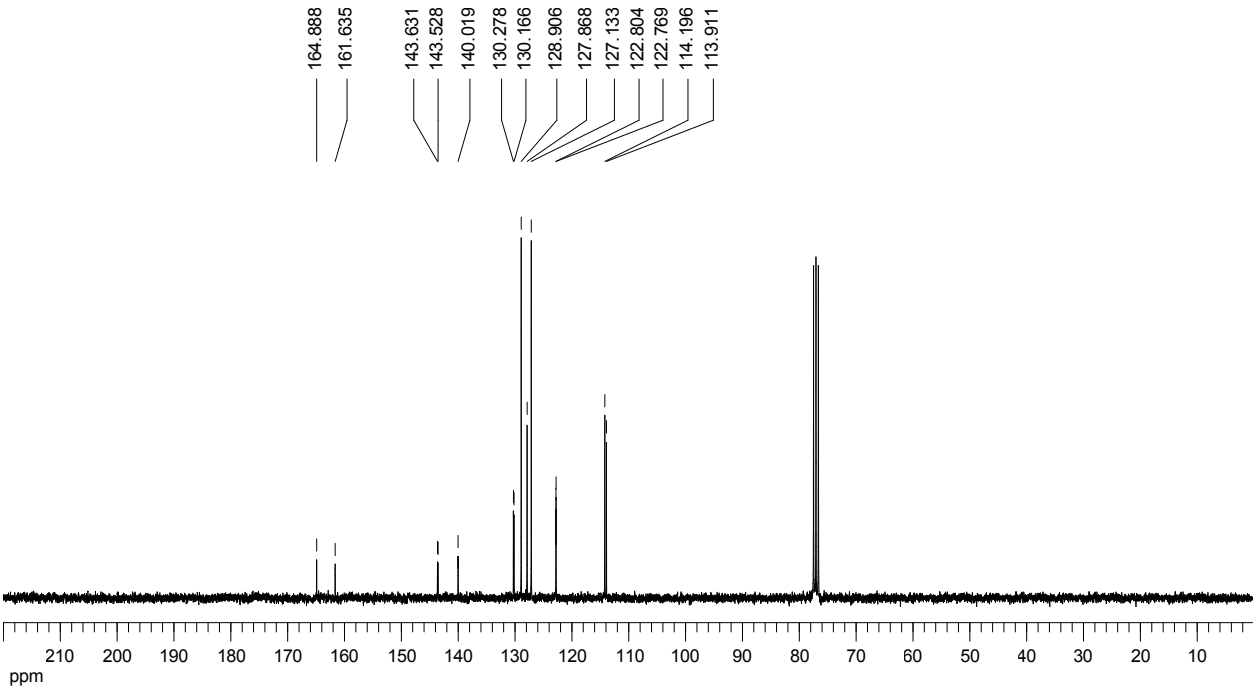
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

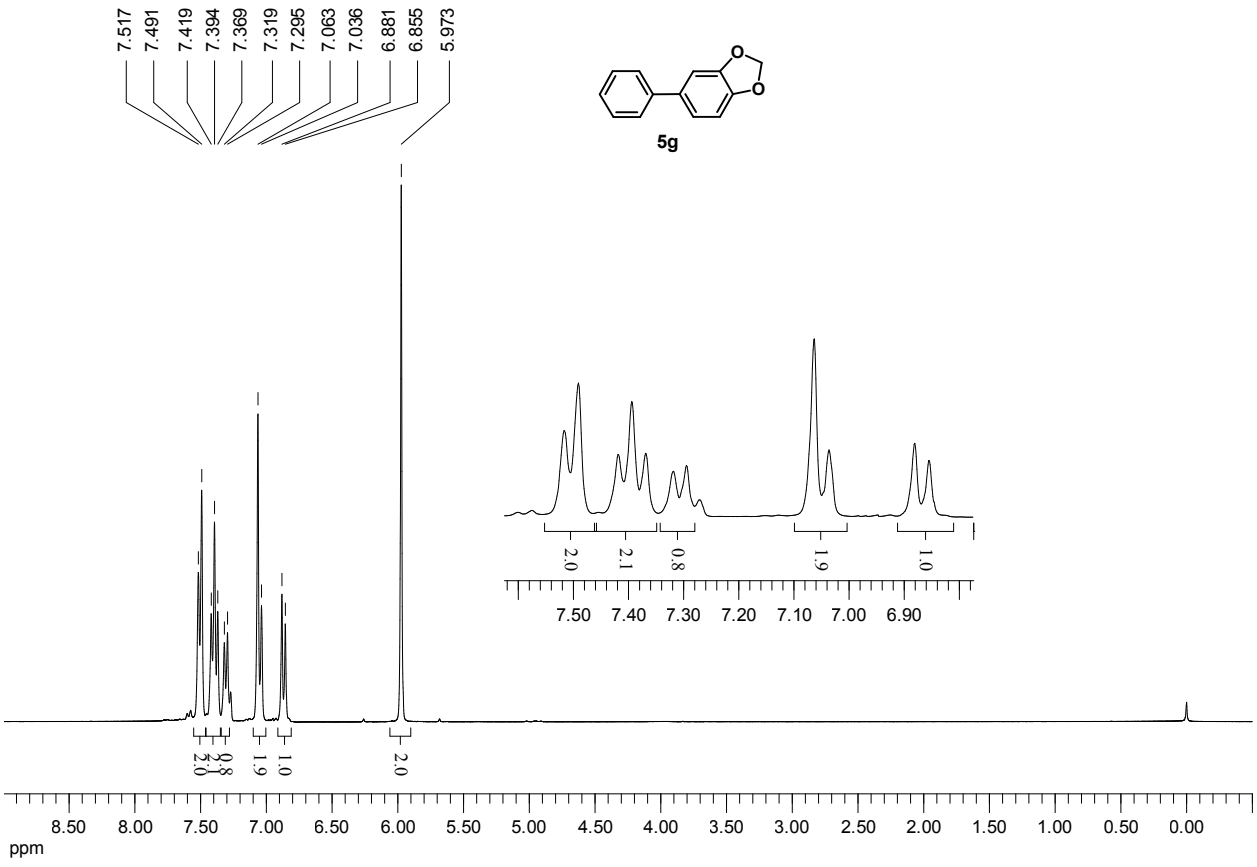

147.808
147.049
138.911
138.770
129.710
129.090
128.135
127.791
124.531
124.059
21.538
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

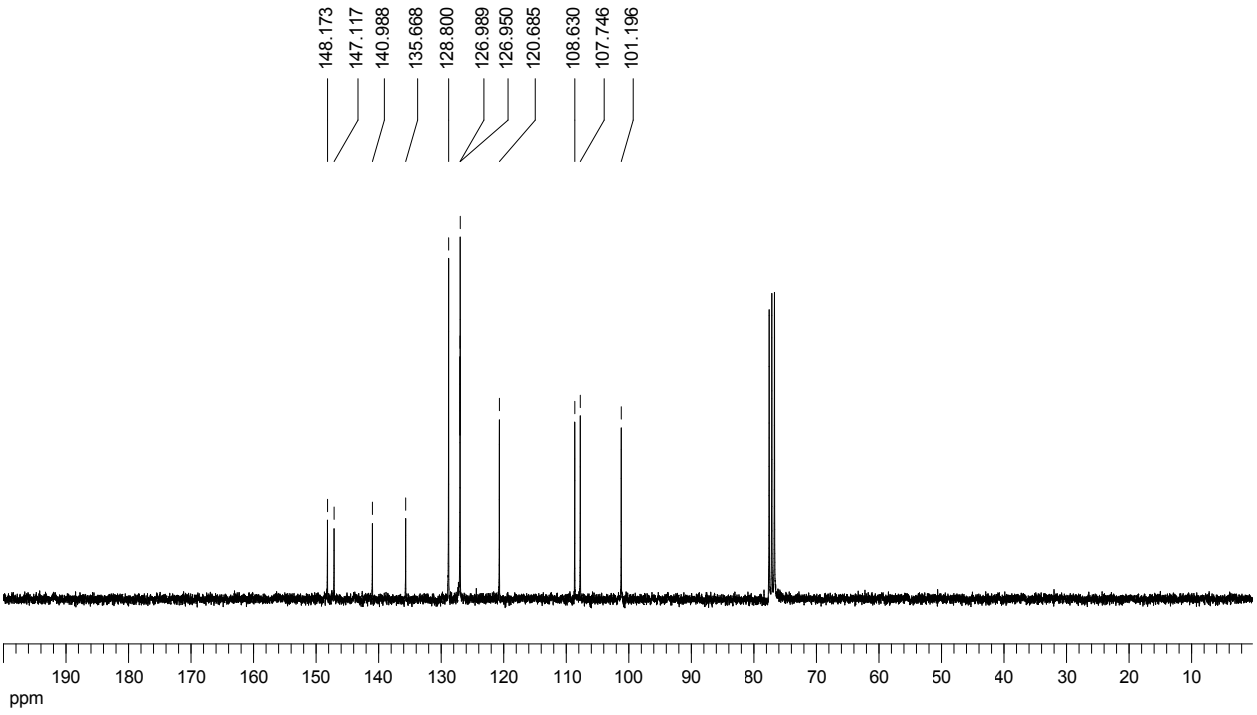

MeO
NO2
5e
8.260
8.231
7.686
7.657
7.583
7.554
7.025
6.996
3.865
1.9
4.0
2.0
8.25
8.00
7.75
7.50
7.25
7.00
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
ppm

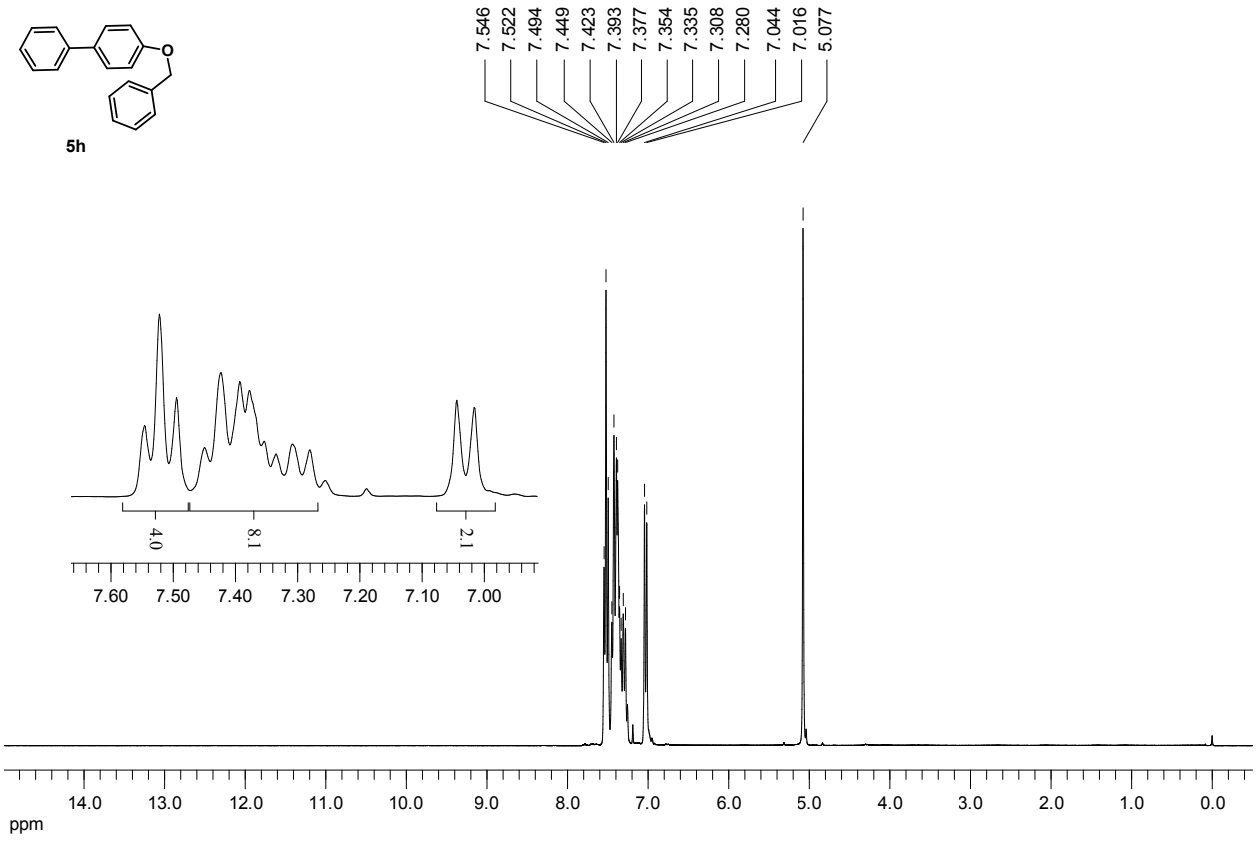

160.484
147.215
146.550
131.060
128.585
127.071
124.154
114.643
55.456
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

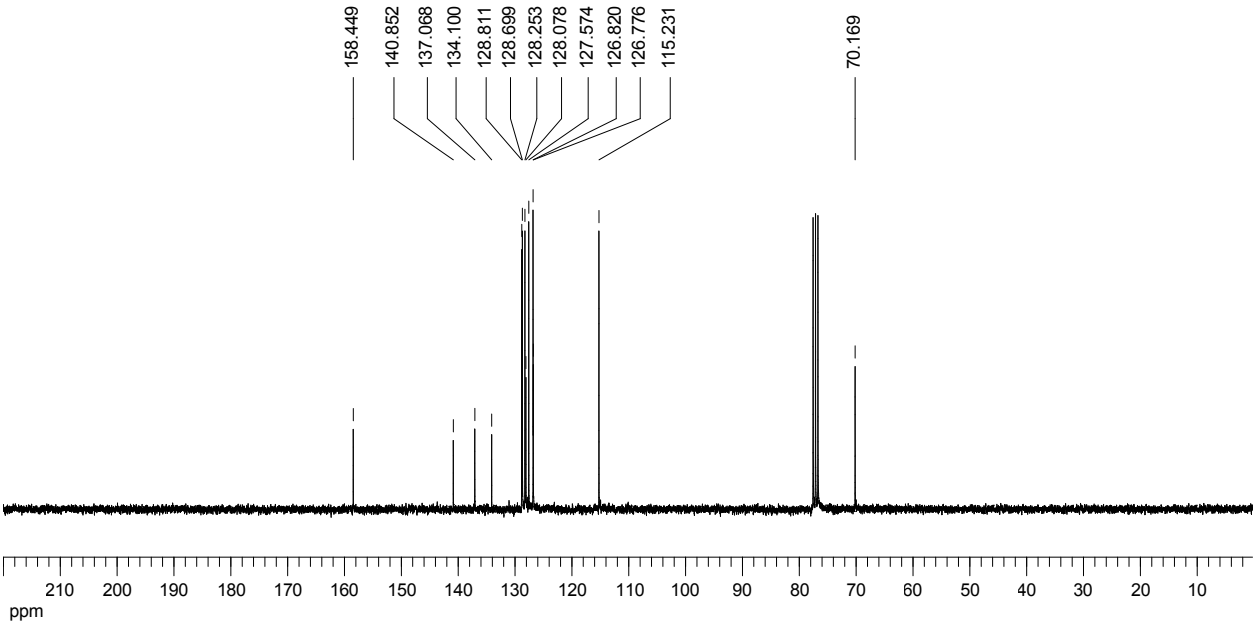

5f
F
7.571
7.547
7.456
7.432
7.407
7.390
7.363
7.353
7.294
7.261
7.235
7.219
7.048
7.019
6.998
6.989
2.0
2.1
3.0
1.1
1.1
7.60
7.50
7.40
7.30
7.20
7.10
7.00
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
ppm

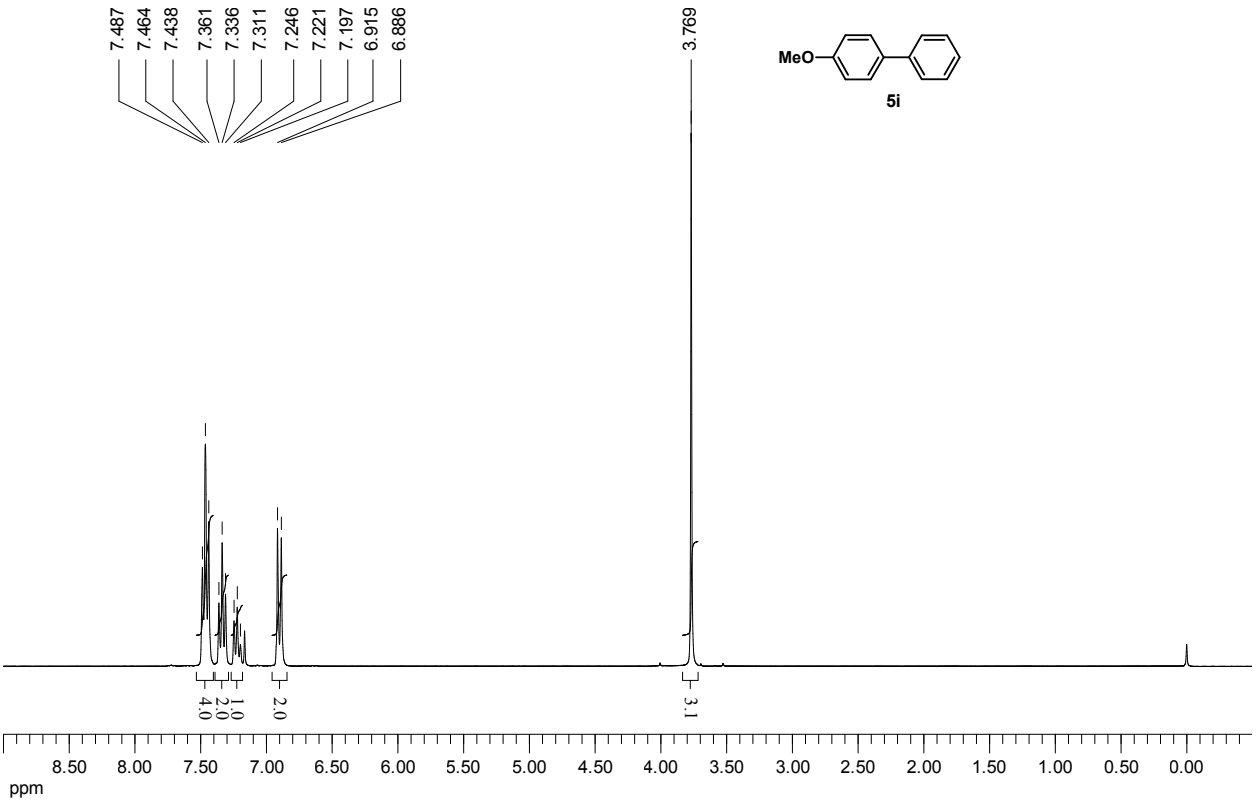

164.888
161.635
143.631
143.528
140.019
130.278
130.166
128.906
127.868
127.133
122.804
122.769
114.196
113.911
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.517
7.491
7.419
7.394
7.369
7.319
7.295
7.063
7.036
6.881
6.855
5.973
5g
2.0
2.1
0.8
1.9
1.0
7.50 7.40 7.30 7.20 7.10 7.00 6.90
2.0
2.1
0.8
1.9
1.0
2.0
8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm


148.173
147.117
140.988
135.668
128.800
126.989
126.950
120.685
108.630
107.746
101.196
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


5h
7.546
7.522
7.494
7.449
7.423
7.393
7.377
7.354
7.335
7.308
7.280
7.044
7.016
5.077
4.0
8.1
2.1
7.60
7.50
7.40
7.30
7.20
7.10
7.00
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


158.449
140.852
137.068
134.100
128.811
128.699
128.253
128.078
127.574
126.820
126.776
115.231
70.169
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.487
7.464
7.438
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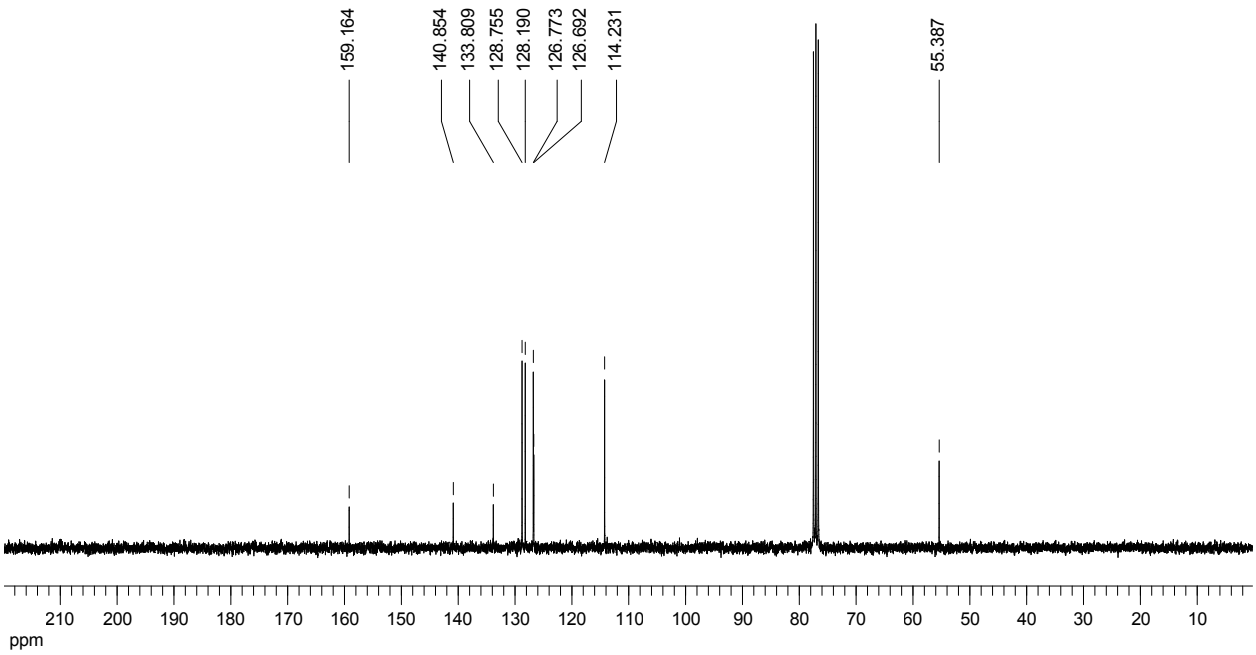
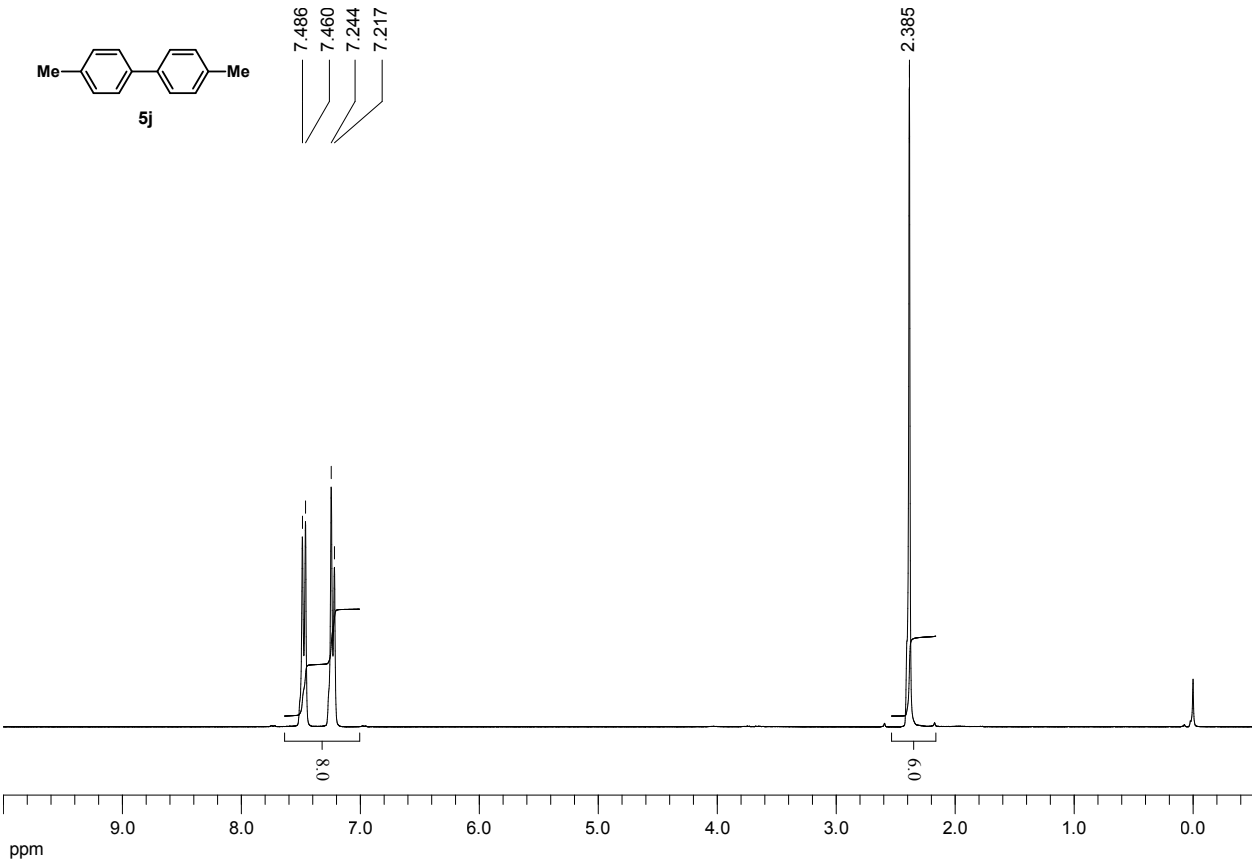
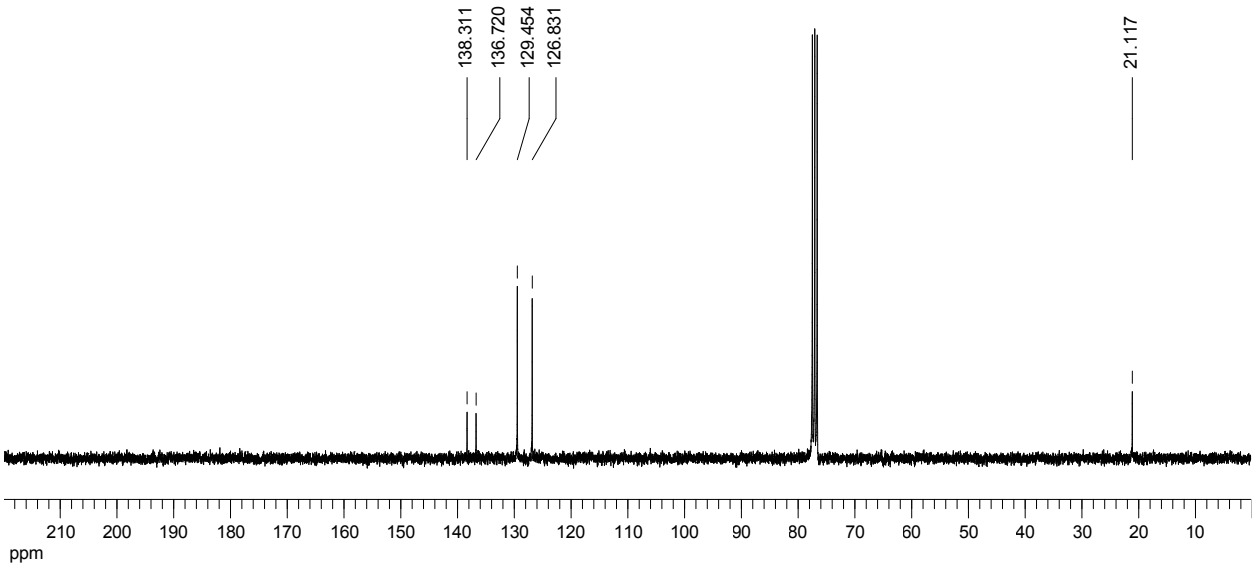
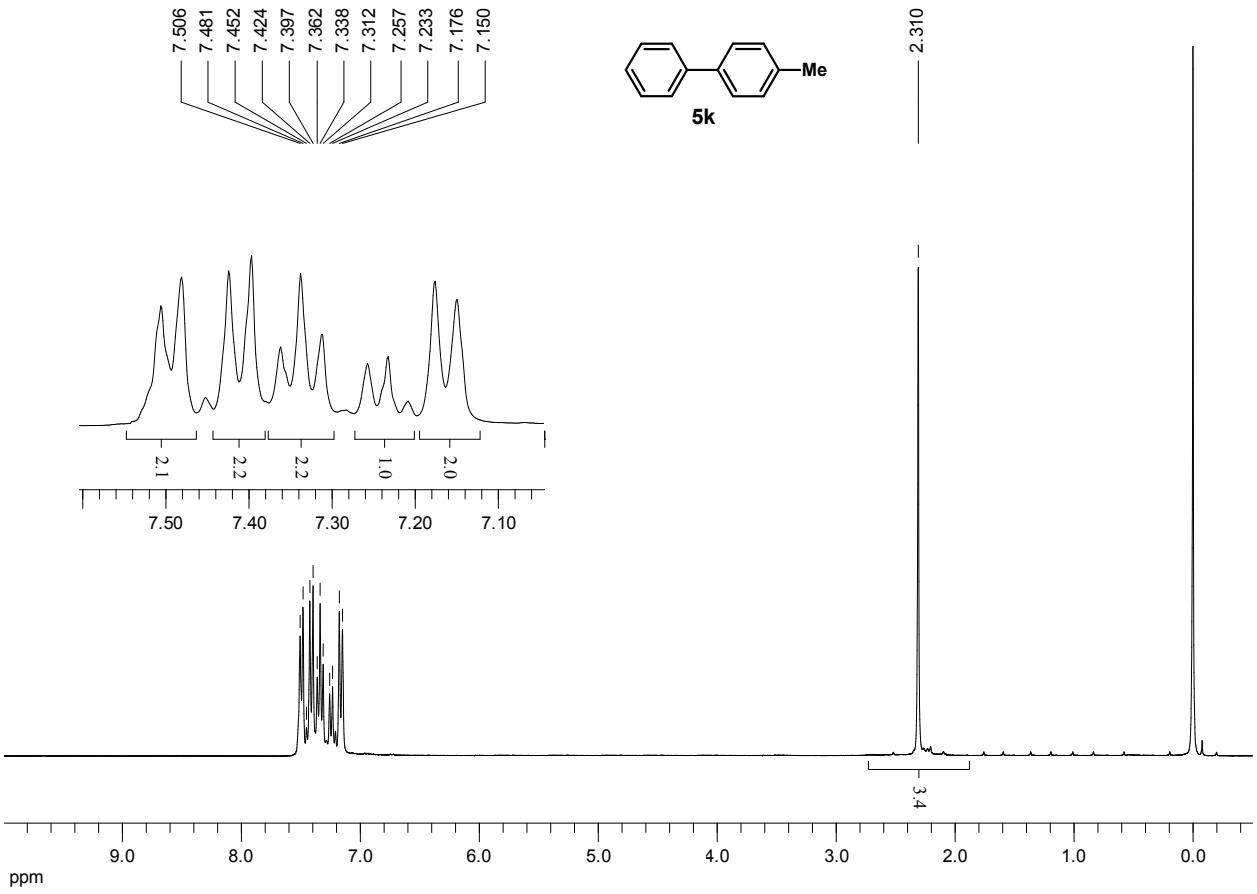
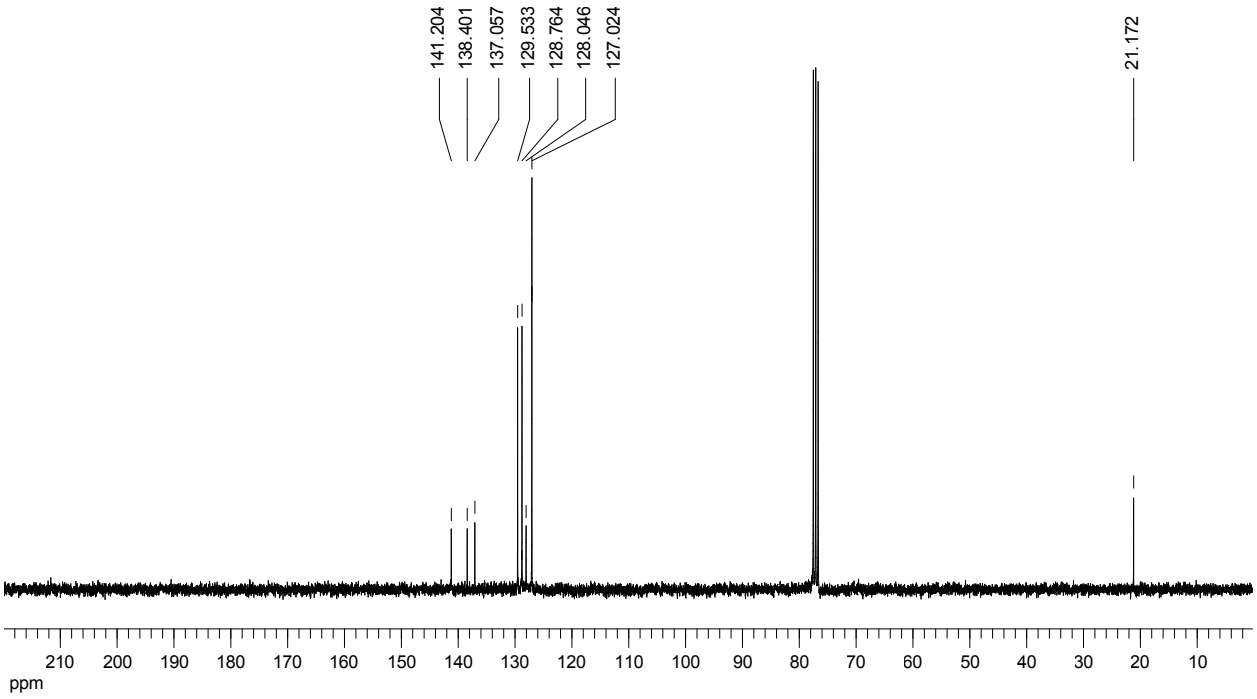
7.336
7.311
7.246
7.221
7.197
6.915
6.886
3.769
MeO
5i
4.0
2.0
1.0
1.0
2.0
3.1
8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 0.00
ppm


159.164
140.854
133.809
128.755
128.190
126.773
126.692
114.231
55.387
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


Me
Me
5j
7.486
7.460
7.244
7.217
2.385
8.0
6.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


138.311
136.720
129.454
126.831
21.117
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.506
7.481
7.452
7.424
7.397
7.362
7.338
7.312
7.257
7.233
7.176
7.150
Me
5k
2.310
2.1
2.2
2.2
1.0
2.0
7.50
7.40
7.30
7.20
7.10
3.4
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


141.204
138.401
137.057
129.533
128.764
128.046
127.024
21.172
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm