Electronic Supplementary Material (ESI) for RSC Advances.

– Supporting Information –

Unexpected Hydrazine Hydrate-Mediated Aerobic Oxidation of Aryl/Heteroaryl boronic Acids to Phenols with Ambient Air

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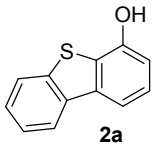
Table of Contents

1. General Procedure for aerobic oxidation of aryl/heteroaryl boronic acids to phenols with ambient Air. A flask was charged with aryl/heteroaryl boronic acid **1** (0.5 mmol), $N_2H_4 \cdot H_2O$ (0.25 mmol, 14.4 μL), Cs_2CO_3 (1.0 mmol, 329.1 mg), H_2O (2.5 mmol, 45.0 μL), and PEG-400 (2.0 g). Then, the flask was stirred at 80 °C in open air for the indicated time. At the end of the reaction, the reaction mixture was acidified with dilute aqueous HCl and extracted with ethyl acetate (3 × 15 mL). The organic phases were combined, and the volatile components were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate).

2. Analytical methods

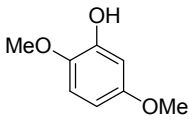
^{1}H and ^{13}C NMR spectra of solutions in $CDCl_3$ or DMSO–d_6 were recorded on a Bruker Avance 400 instrument. Chemical shifts were expressed in parts per million (ppm) downfield from tetramethylsilane and refer to the solvent signals ($CDCl_3$: H 7.24 and C 77.0 ppm; DMSO-d_6 : H 2.50 and C 39.5 ppm). The signals of water were observed at about 1.58 ppm and 3.34 ppm in $CDCl_3$ and DMSO-d_6, respectively. Abbreviations for signal couplings are: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet; dd, doublet of doublets; dt, triplet of doublets; td, doublet of triplets; tt, triplet of triplets; ddd, doublet of doublet of doublets; tdd, doublet of doublet of triplets. Coupling constants, *J,* were reported in hertz unit (Hz).

3. Analytical data of products



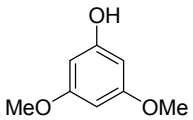
2a

Dibenzothiophen-4-ol (2a): Following general procedure, **2a** was isolated as a light pink solid (86% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.5 (br s, 1 H), 8.29−8.26 (m, 1 H), 8.02−7.99 (m, 1 H), 7.80 (dd, J = 8.0, 4.0 Hz, 1 H), 7.52−7.45 (m, 2 H), 7.34 (t, J = 8.0 Hz, 1 H), 6.95 ppm (dd, J = 8.0, 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 152.3, 138.7, 136.9, 135.7, 126.9, 126.2, 125.6, 124.6, 123.2, 122.2, 112.9, 111.5 ppm; mp 166.3−167.1 °C (lit.[S1] mp 158-160 °C).



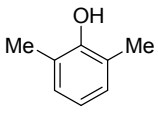
2b

2,5-Dimethoxyphenol (2b): Following general procedure, **2b** was isolated as a light yellow liquid (91% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S2] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.75 (d, J = 8.0 Hz, 1 H), 6.54 (d, J = 4.0 Hz, 1 H), 7.64 (dd, J = 8.0, 4.0 Hz, 1 H), 5.65 (s, 1 H), 3.82 (s, 3 H), 3.73 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 146.4, 140.9, 111.4, 104.2, 101.7, 56.6, 55.6 ppm.



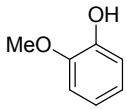
2c

3,5-Dimethoxyphenol (2c): Following general procedure, **2c** was isolated as a light brown oil. (92% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S3] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.04 (t, J = 2.0 Hz, 1 H), 6.02 (d, J = 2.0 Hz, 2 H), 4.73 (br s, 1 H), 3.71 ppm (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 157.6, 94.3, 92.9, 55.3 ppm.



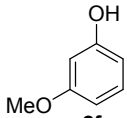
2d

2,6-Dimethylphenol (2d): Following general procedure A, **2d** was isolated as a white solid (96% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.96 (d, J = 8.0 Hz, 2 H), 6.74 (t, J = 8.0 Hz, 1 H), 4.58 (br s, 1 H), 2.24 ppm (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.1, 128.6, 122.9, 120.2, 15.8 ppm; mp 42.8−44.2 °C (lit.[S1] mp 43-45 °C).



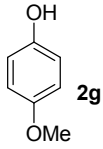
2e

2-Methoxyphenol (2e): Following general procedure, **2e** was isolated as a light yellow oil (97% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.94−6.91 (m, 1 H), 6.89−6.84 (m, 3 H), 5.64 (br s, 1 H), 3.87 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.5, 145.6, 121.4, 120.1, 114.5, 110.7, 55.8 ppm.



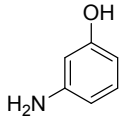
2f

3-Methoxyphenol (2f): Following general procedure, **2f** was isolated as a light yellow oil (83% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.11 (t, J = 8.0 Hz, 1 H), 6.49−6.30 (m, 3 H), 4.14 (br s, 1 H), 3.76 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.9, 156.9, 130.1, 107.9, 106.3, 101.6, 55.3 ppm.



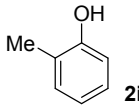
2g

4-Methoxyphenol (2g): Following general procedure, **2g** was isolated as a low melting point solid (98% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.79−6.73 (m, 4 H), 4.86 (br s, 1 H), 3.75 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 149.4, 116.0, 114.8, 55.8 ppm.



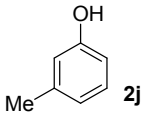
2h

3-Aminophenol (2h): Following general procedure, **2h** was isolated as a white solid (85% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S4] ^{1}H NMR (400 MHz, DMSO-d_3): δ 8.86 (br s, 1 H), 6.80−6.76 (m, 1 H), 6.02−6.00 (m, 2 H), 5.96−5.93 (m, 1 H), 4.92 ppm (br s, 2 H); ^{13}C NMR (100 MHz, DMSO-d_3): δ 158.1, 149.8, 129.5, 105.6, 103.5, 101.1 ppm; mp 118.8−120.2 °C (lit.[S4] mp 120−121 °C).



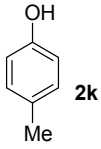
2i

2-Methylphenol (2i): Following general procedure, **2i** was isolated as a low melting point solid (91% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S5] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13−7.06 (m, 2 H), 6.85 (td, J = 8.0, 0.8 Hz, 1 H), 6.76 (d, J = 8.0 Hz, 2 H), 4.78 (br s, 1 H), 2.25 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 131.0, 127.1, 123.7, 120.7, 114.8, 15.7 ppm.



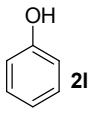
2j

3-Methylphenol (2j): Following general procedure, **2j** was isolated as a colorless oil (95% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S6] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (t, *J* = 8.0 Hz, 1 H), 6.76 (d, *J* = 8.0 Hz, 1 H), 6.67−6.64 (m, 2 H), 4.89 (br s, 1 H), 2.30 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 139.8, 129.4, 121.6, 116.0, 112.3, 21.3 ppm.



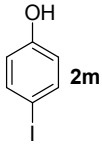
2k

4-Methylphenol (2k): Following general procedure, **2k** was isolated as a low melting point solid (90% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S6] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02−6.91 (dd, *J* = 8.0, 0.8 Hz, 2 H), 6.72 (d, *J* = 8.0 Hz, 2 H), 4.49 (br s, 1 H), 2.26 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.2, 130.0, 129.9, 115.0, 20.4 ppm.



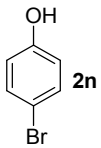
2l

Phenol (2l): Following general procedure A, **2l** was isolated as a white yellow solid (87% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (t, *J* = 8.0 Hz, 2 H), 6.93 (t, *J* = 8.0 Hz, 1 H), 6.83 (d, *J* = 8.0 Hz, 2 H), 4.84 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 129.7, 120.8, 115.3 ppm; mp 41.2−42.6 °C (lit.[S1] mp 40-42 °C).



2m

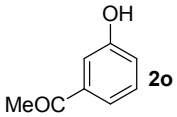
4-Iodophenol (2m): Following general procedure A, **2m** was isolated as a light yellow solid (98% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, *J* = 8.0 Hz, 2 H), 6.61 (d, *J* = 8.0 Hz, 2 H), 5.03 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 138.4, 117.8, 82.7 ppm; mp 63.3−64.2 °C (lit.[S1] mp 90−93 °C).



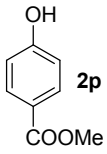
2n

4-Bromophenol (2n): Following general procedure, **2n** was isolated as a light yellow solid (96%

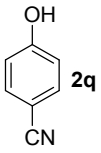
yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (d, *J* = 8.0 Hz, 2 H), 6.71 (d, *J* = 8.0 Hz, 2 H), 4.83 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.6, 132.4, 117.2, 112.9 ppm; mp 54.3−56.2 °C (lit. [S1] mp 55−58 °C).



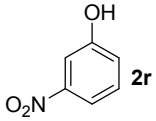
3-Hydroxyacetophenone (2o): Following general procedure, **2o** was isolated as a white solid (95% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S7] ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.79 (s, 1 H), 7.41 (dt, *J* = 8.0, 4.0 Hz, 1 H), 7.32 (t, *J* = 8.0 Hz, 2 H), 7.03 (ddd, *J* = 8.0, 4.0, 2.0 Hz, 1 H), 2.52 ppm (s, 3 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 197.8, 157.6, 138.3, 129.8, 120.3, 119.3, 114.3, 26.8 ppm; mp 85.8−86.2 °C (lit.[S7] mp 92−95 °C).



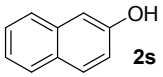
Methyl 4-Hydroxybenzoate (2p): Following general procedure, **2p** was isolated as a white solid (97% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.0 Hz, 2 H), 6.84 (d, *J* = 8.0 Hz, 2 H), 5.51 (br s, 1 H), 3.87 ppm (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.3, 160.1, 131.9, 122.4, 115.2, 52.0 ppm; mp 112.0−113.1 °C (lit. [S1] mp 121−123 °C).



4-Hydroxybenzonitrile (2q): Following general procedure, **2q** was isolated as a light yellow solid (98% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, *J* = 8.0 Hz, 2 H), 6.92 (d, *J* = 8.0 Hz, 2 H), 6.34 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 134.3, 119.3, 116.5, 102.8 ppm; mp 109.1−111.2 °C (lit.[S1] mp 107−109 °C)..

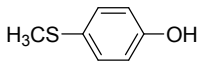


3-Nitrophenol (2r): Following general procedure, **2r** was isolated as a light yellow solid (89% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (ddd, *J* = 8.0, 4.0, 2.0 Hz, 1 H), 7.70 (t, *J* = 8.0 Hz, 1 H), 7.39 (t, *J* = 8.0, 4.0, 2.0 Hz, 1 H), 7.19 (ddd, *J* = 8.0, 4.0, 2.0 Hz, 1 H), 5.97 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 149.0, 130.3, 122.1, 115.9, 110.5 ppm; mp 99.0−100.1 °C(lit.[S1] mp 96−99 °C).



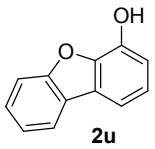
2s

2-Napthol (2s): Following general procedure, **2s** was isolated as a white solid (97% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (t, *J* = 8.0 Hz, 2 H), 7.66 (d, *J* = 8.0 Hz, 1 H), 7.44−7.40 (m, 1 H), 7.34−7.30 (m, 1 H), 7.13 (d, *J* = 4.0 Hz, 1 H), 7.11 (td, *J* = 8.0, 4.0 Hz, 2 H), 4.86 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.3, 134.6, 129.8, 128.9, 127.7, 126.5, 126.4, 123.6, 117.7, 109.5 ppm; mp 116.0−116.8 °C (lit.[S1] mp 121−123 °C).



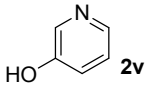
2t

4-(Methylmercapto)phenol (2t): Following general procedure A, **2t** was isolated as a white solid (85% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S8] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20 (d, *J* = 8.4 Hz, 2 H), 6.77 (d, *J* = 8.4 Hz, 2 H), 5.18 (br s, 1 H), 2.42 ppm (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.0, 130.3, 128.8, 116.1, 18.0 ppm; mp 83.4-84.3 °C (lit.[S8] mp 83-85 °C).



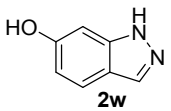
2u

Dibenzofuran-4-ol (2u): Following general procedure, **2u** was isolated as a white solid (83% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.0 Hz, 1 H), 7.57 (d, *J* = 8.0 Hz, 1 H), 7.51 (dd, *J* = 8.0, 4.0 Hz, 1 H), 7.45 (td, *J* = 8.0, 2.0 Hz, 1 H), 7.34 (td, *J* = 8.0, 2.0 Hz, 1 H), 7.21 (t, *J* = 8.0 Hz, 1 H), 7.02 (dd, *J* = 8.0, 4.0 Hz, 1 H), 5.49 ppm (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.0, 144.0, 141.1, 127.3, 125.7, 124.6, 123.7, 122.9, 121.0, 113.6, 112.8, 111.8 ppm; mp 98.2−100.1 °C (lit.[S1] mp 98−100 °C).



2v

Pyridin-3-ol (2v): Following general procedure, **2v** was isolated as a white solid (91% yield), known compound. The NMR spectroscopic data agree with those described in ref..[S7] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, *J* = 4.0 Hz, 1 H), 8.08 (dd, *J* = 8.0, 4.0 Hz, 1 H), 7.32−7.25 ppm (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.1, 139.3, 136.5, 125.2, 125.1 ppm; mp 125.0−126.2 °C (lit.[S7] mp 127 °C).



2w

1*H*-indazol-6-ol (2w): Following general procedure, **2w** was isolated as a light yellow solid (96% yield), known compound (CAS: 23244-88-4). ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.58 (br s, 1 H),

9.57 (br s, 1 H), 7.86 (s, 1 H), 7.52 (d, J = 8.0 Hz, 1 H), 6.78 (s, 1 H), 6.64 ppm (dd, J = 8.0, 2.0 Hz, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 156.5, 141.5, 133.3, 121.1, 117.0, 112.3, 93.2 ppm; mp 161.8−164.2 °C.

4. References

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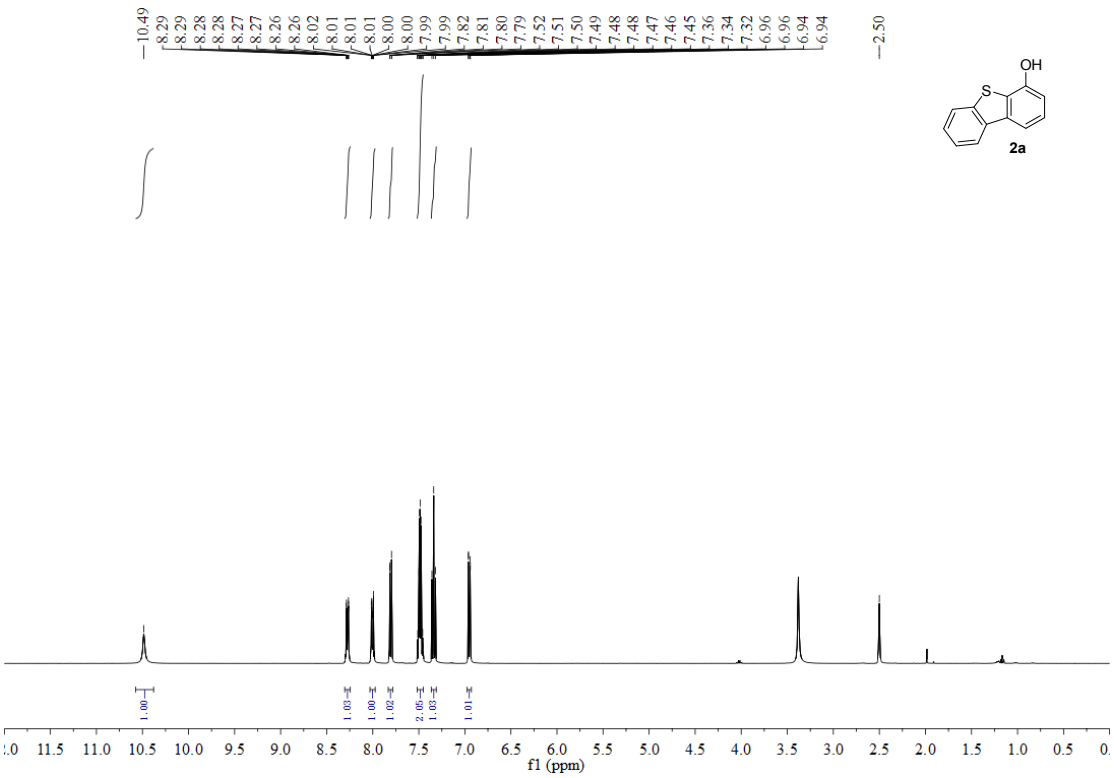
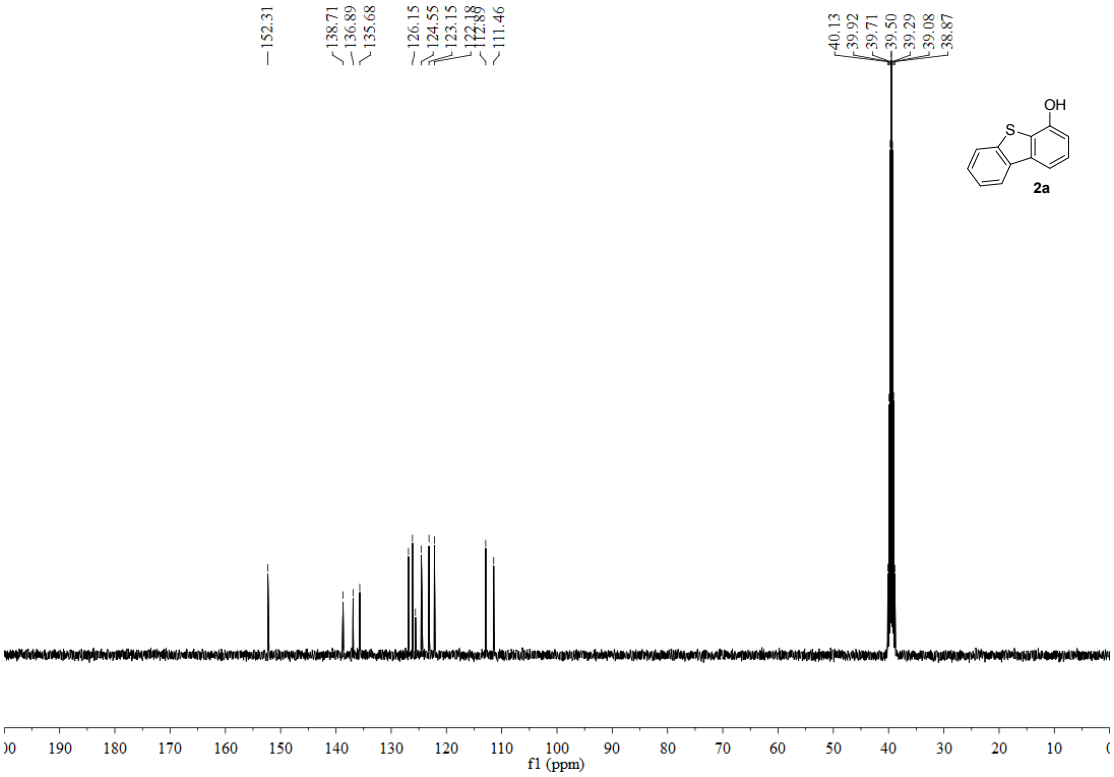
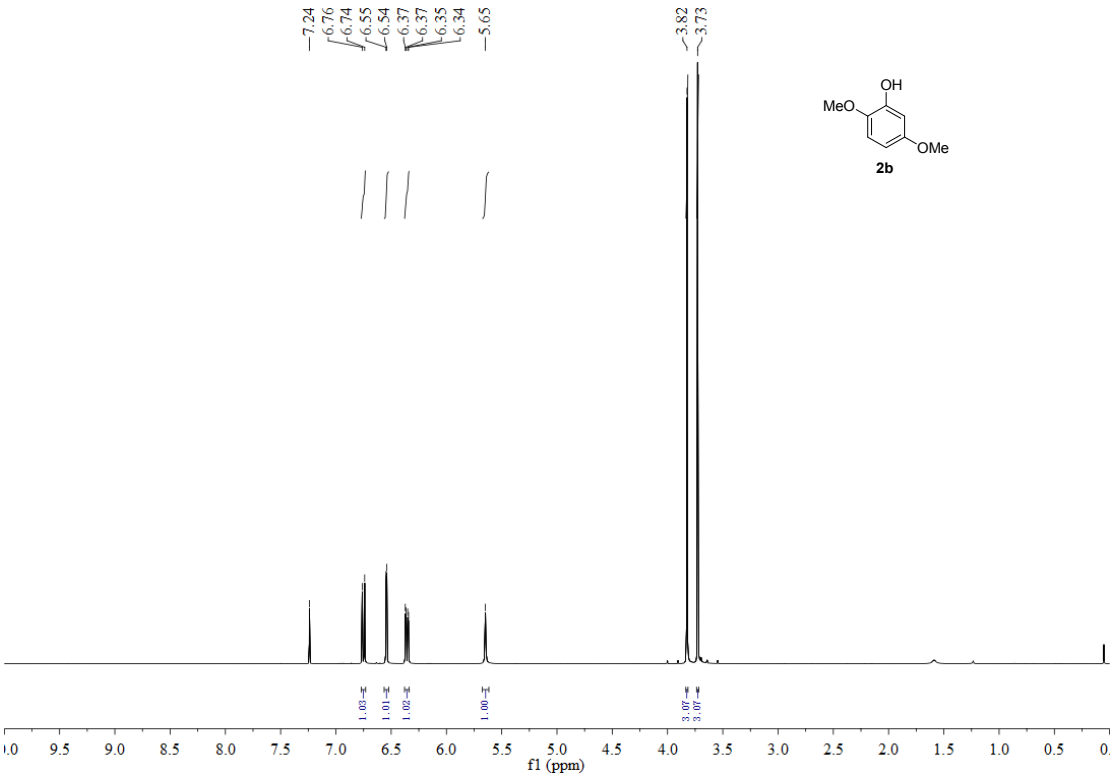
5. Copies of NMR Spectra



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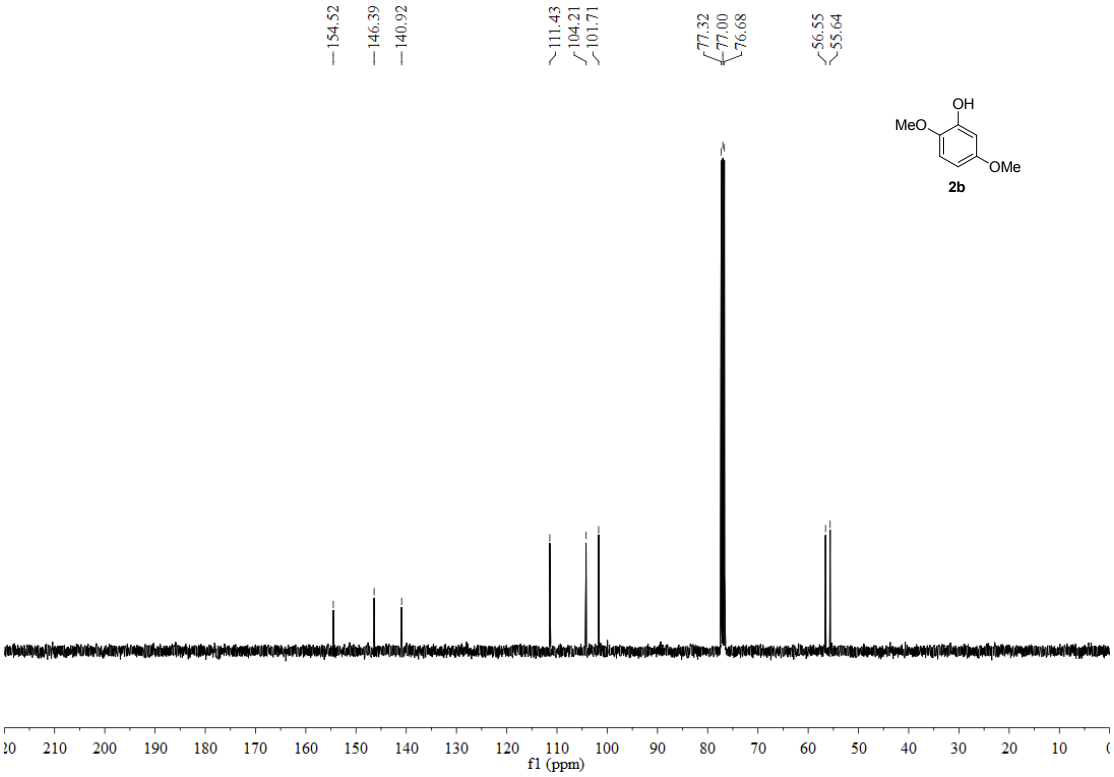
MeO
OMe
2b
1.03
1.01
1.02
1.00
3.07
3.07
f1 (ppm)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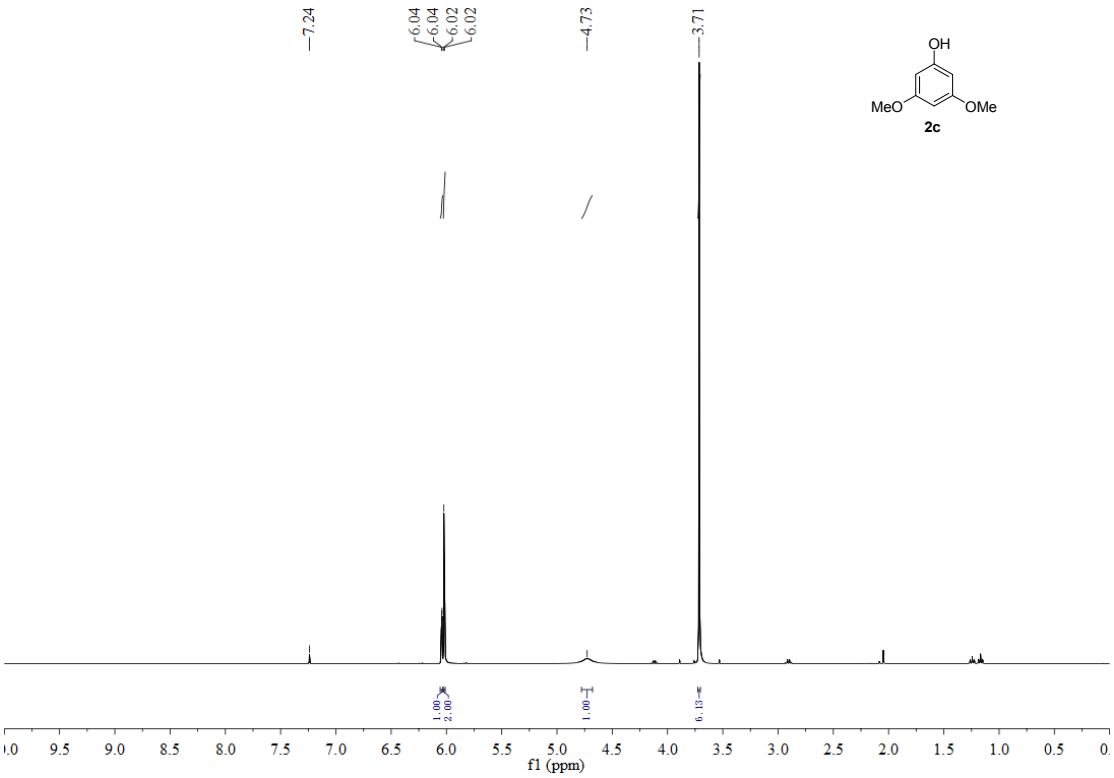
MeO
OMe
2b
f1 (ppm)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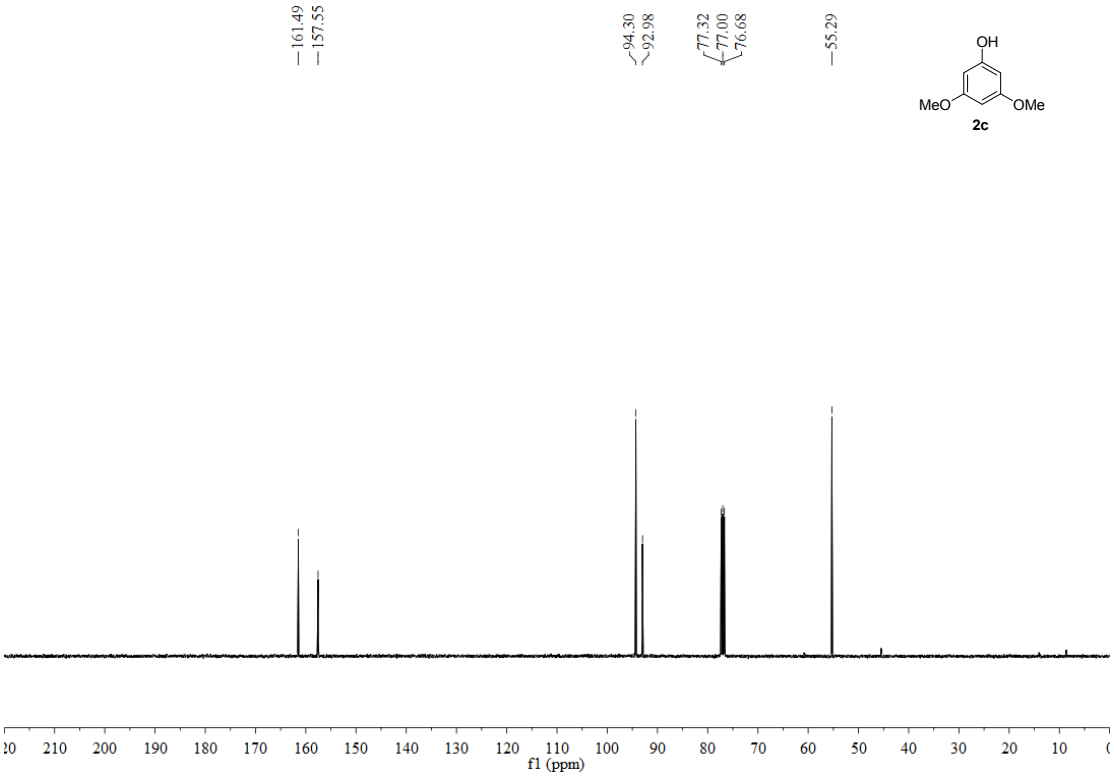
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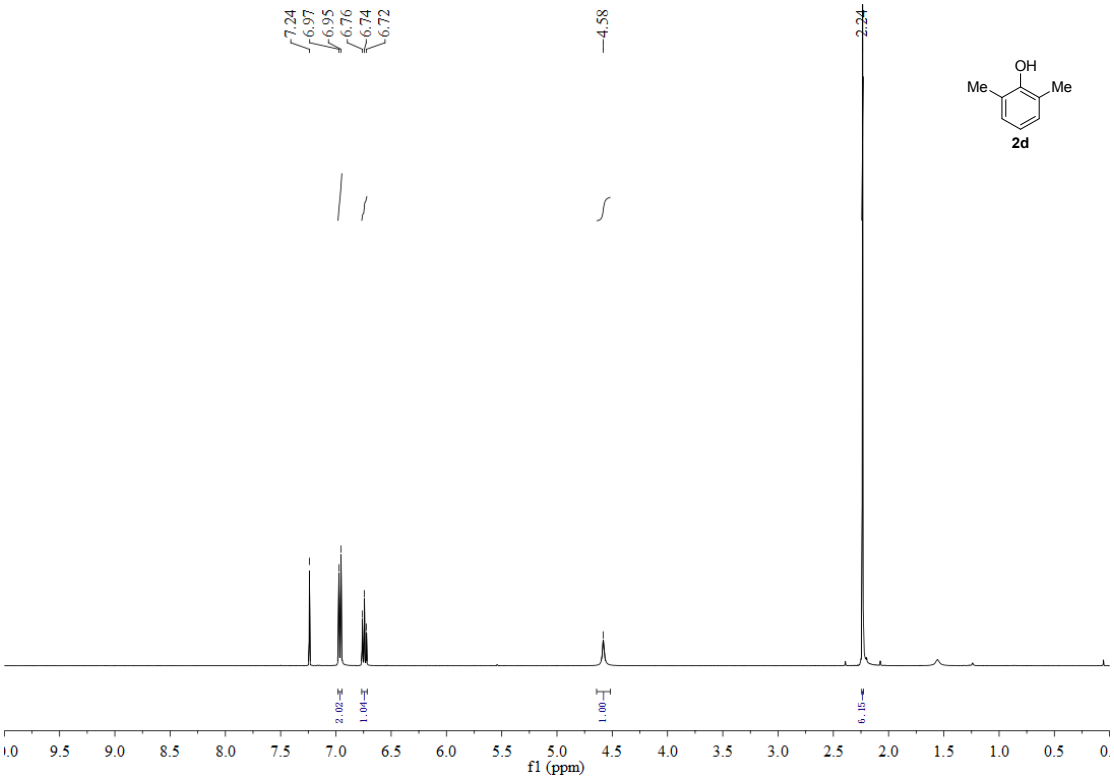
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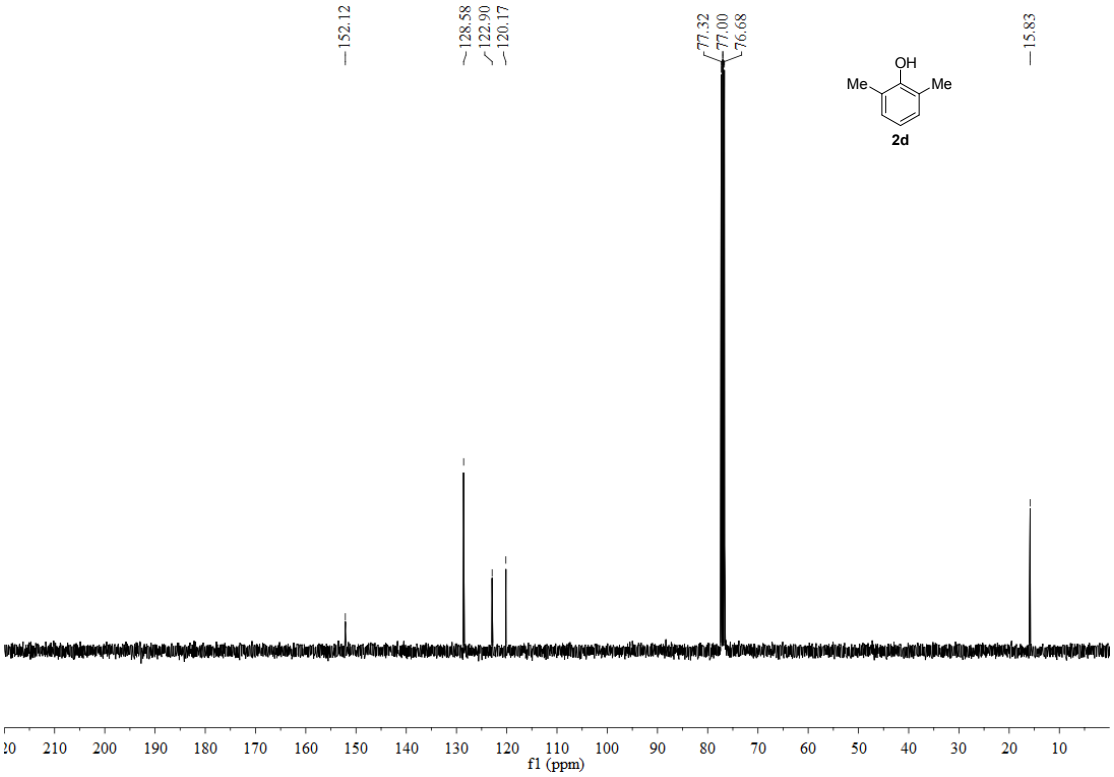
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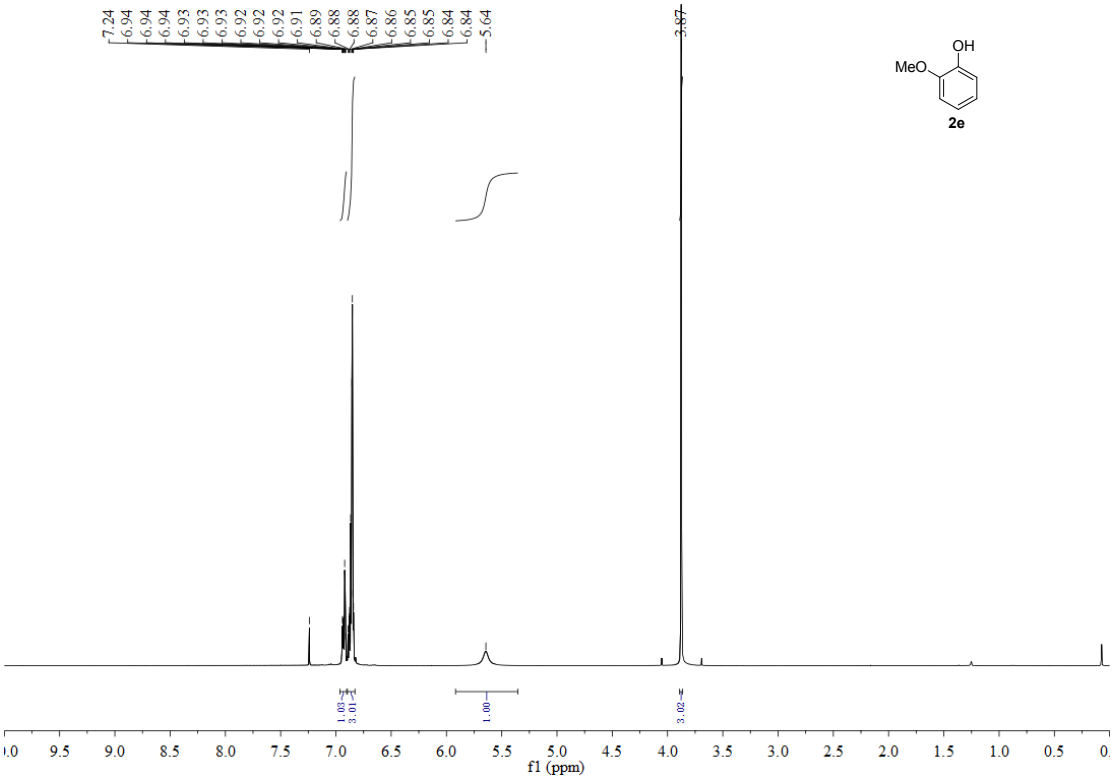
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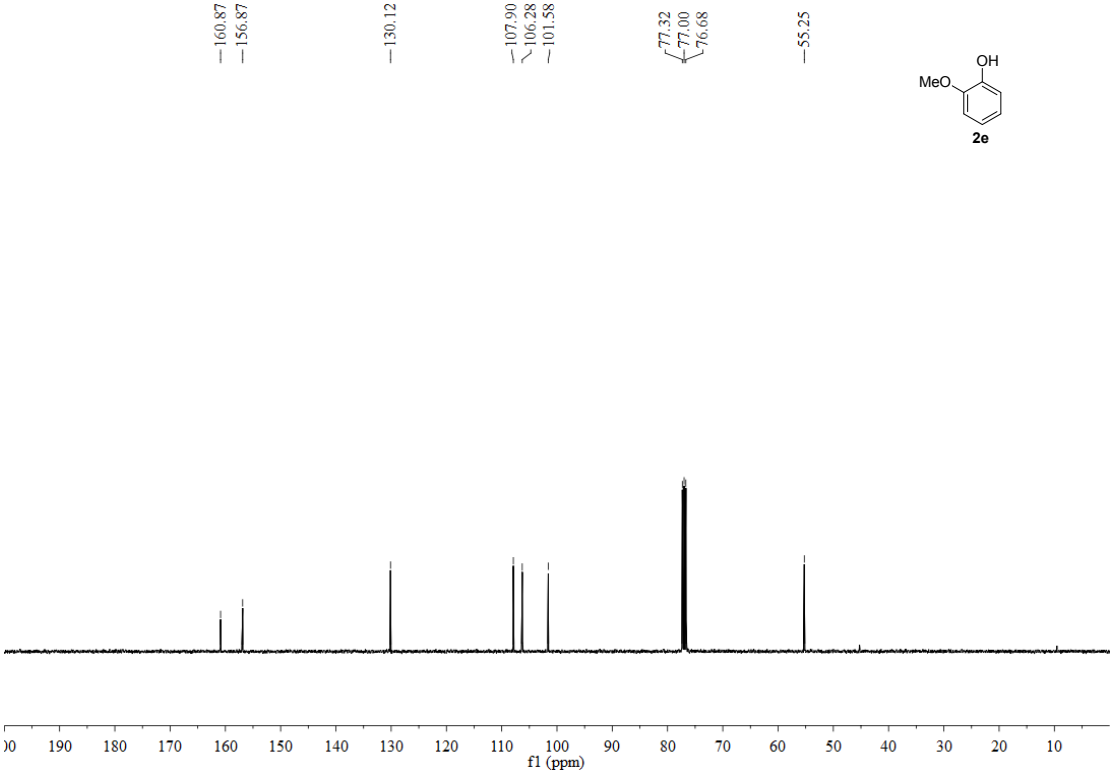
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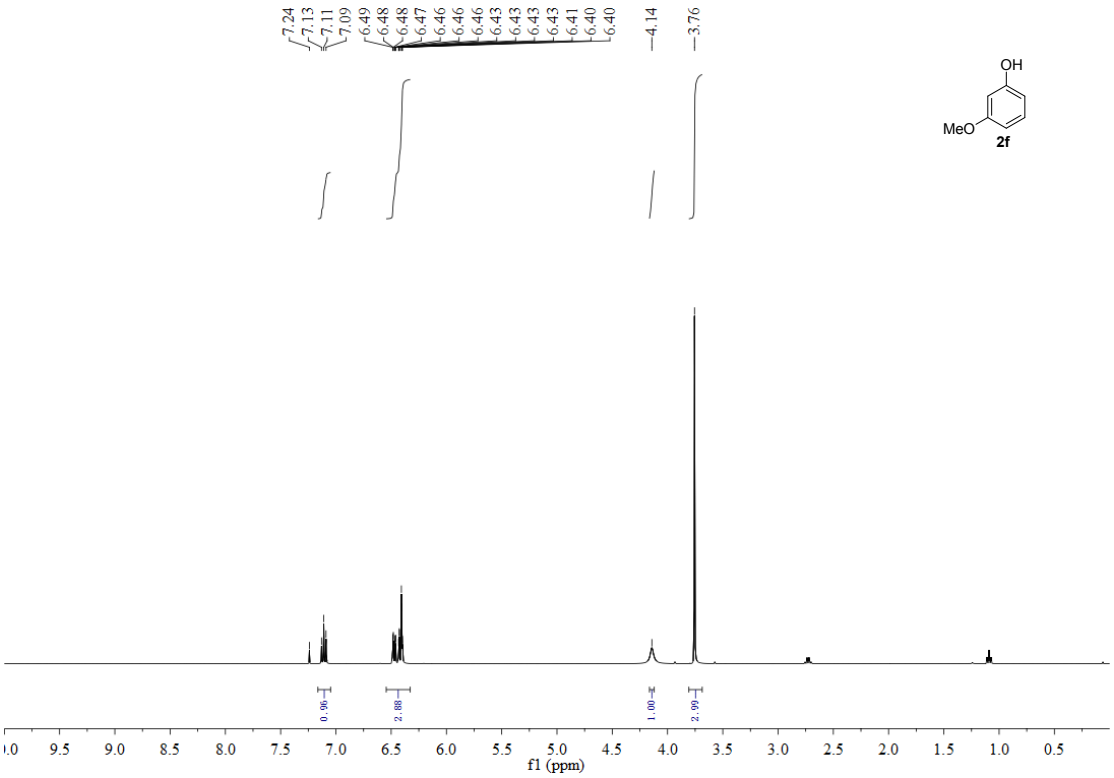
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6.43
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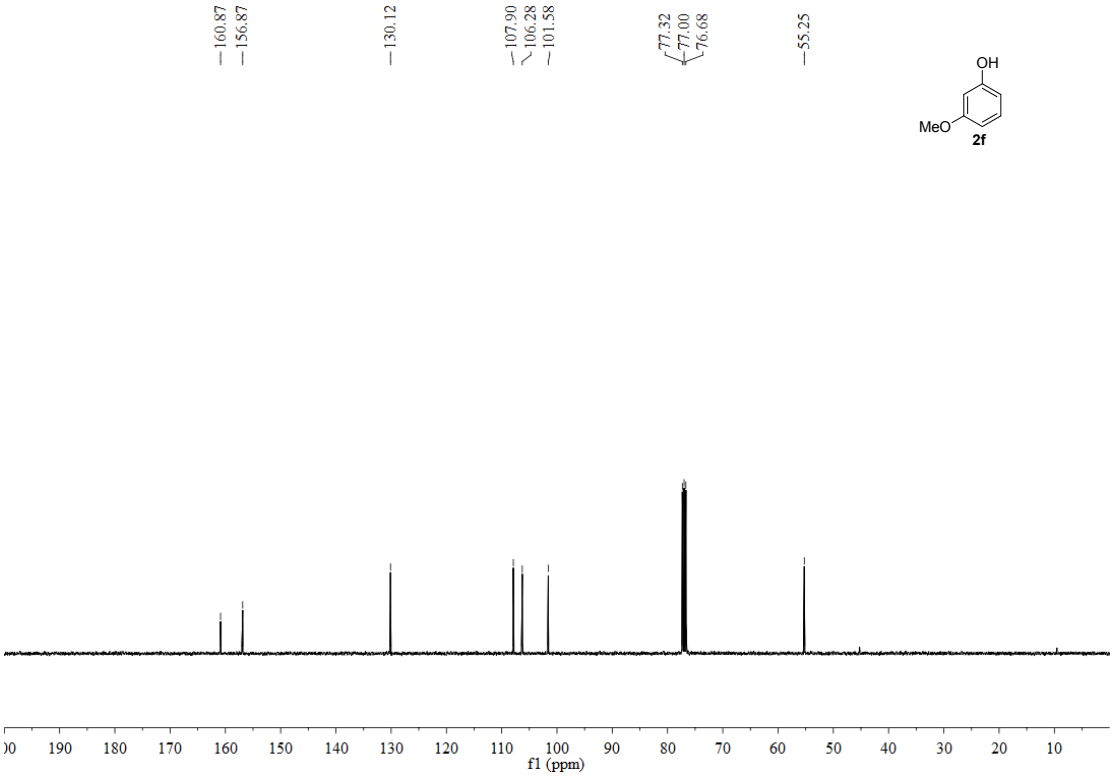
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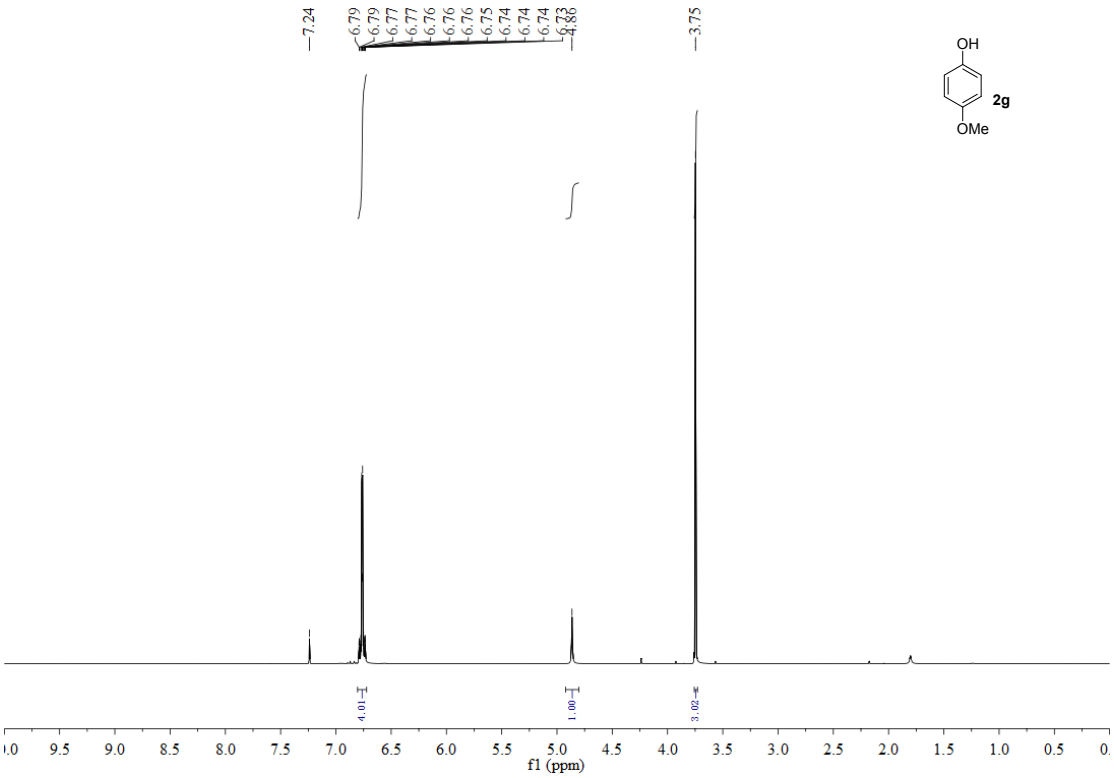
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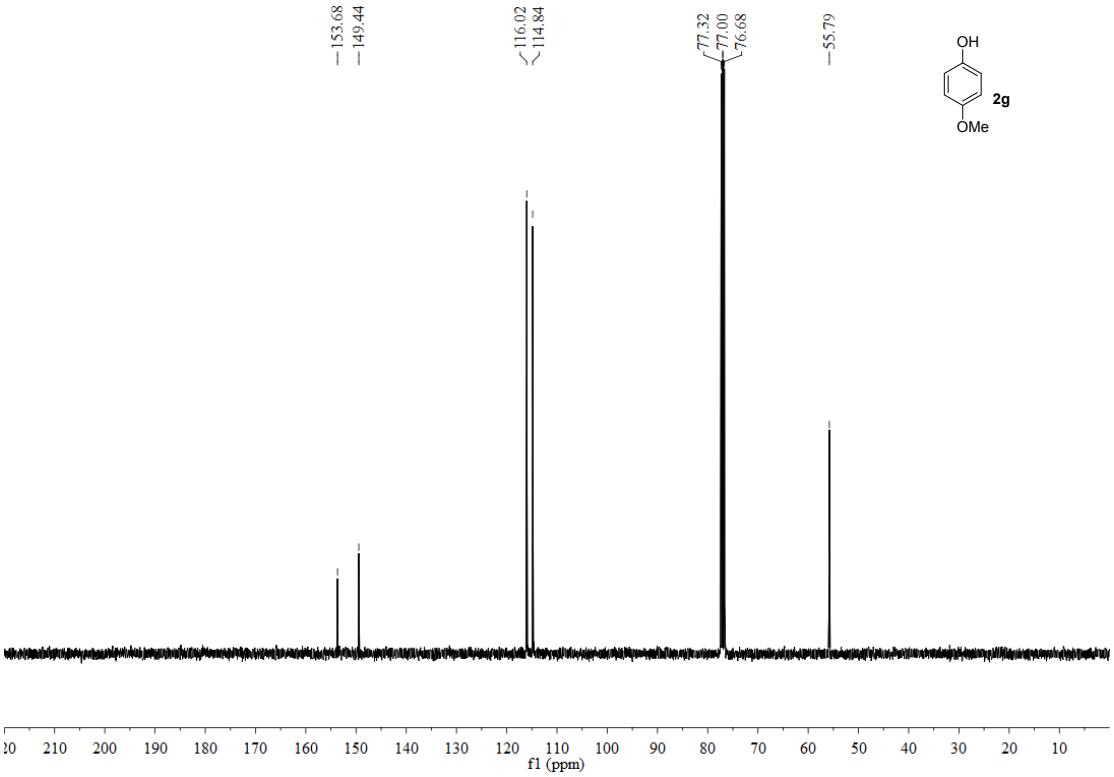
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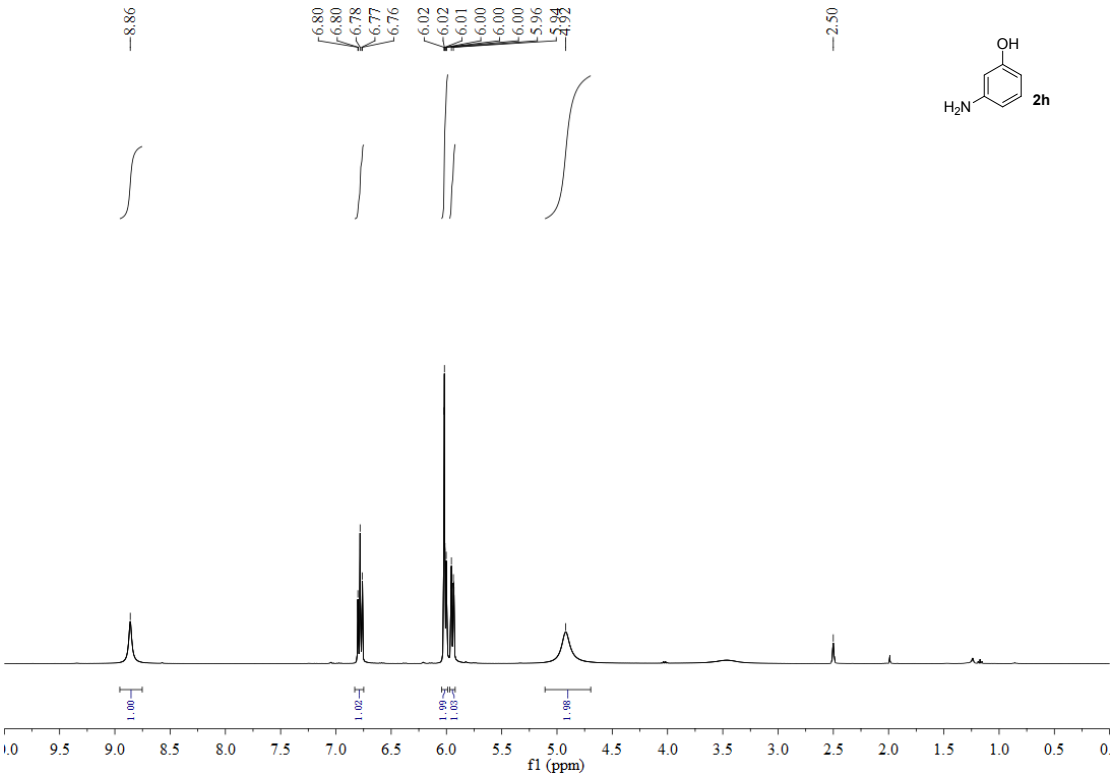
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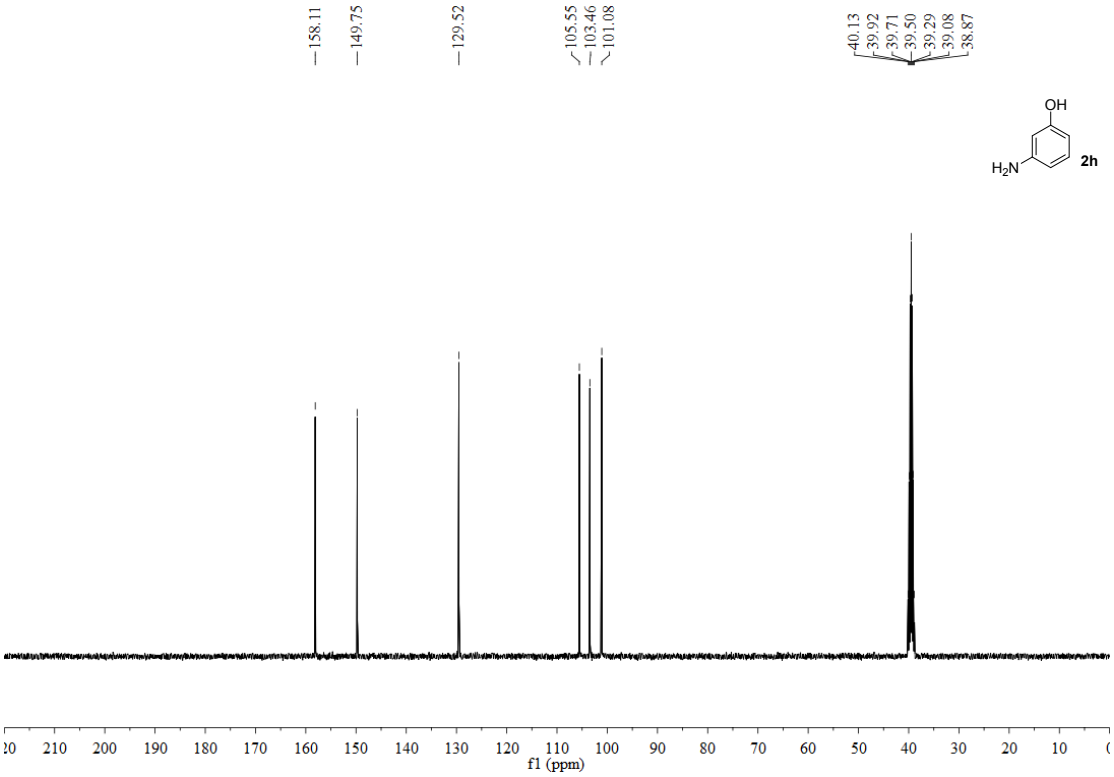
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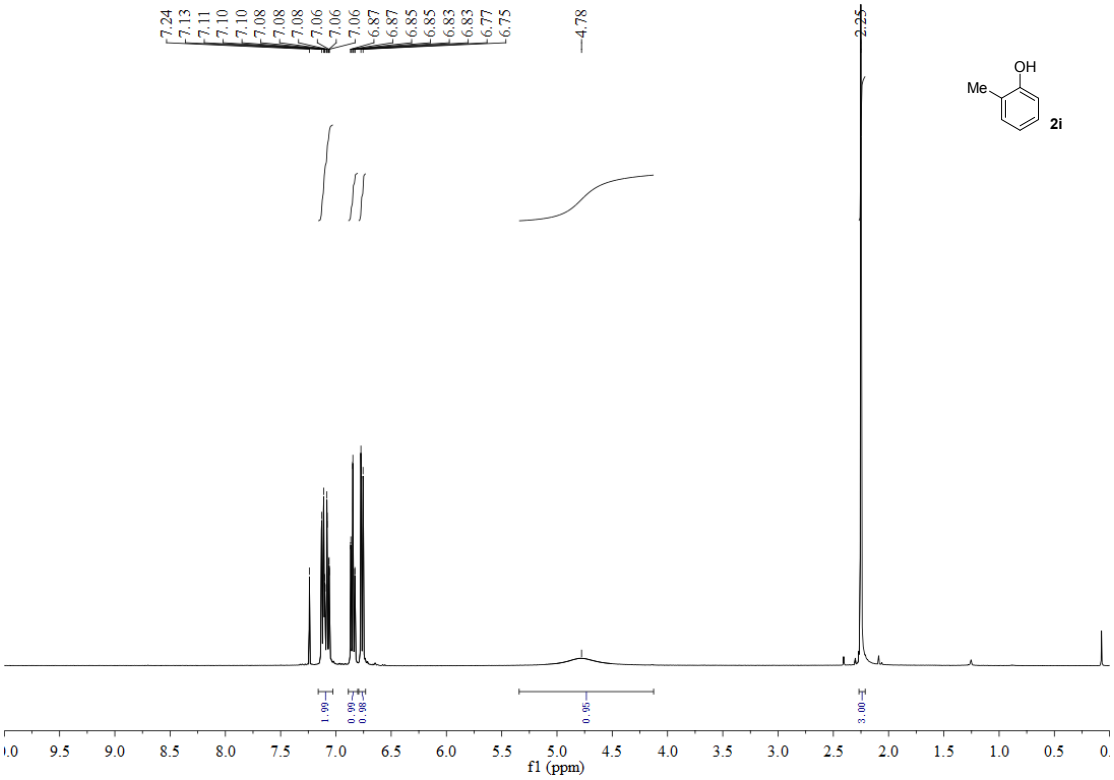
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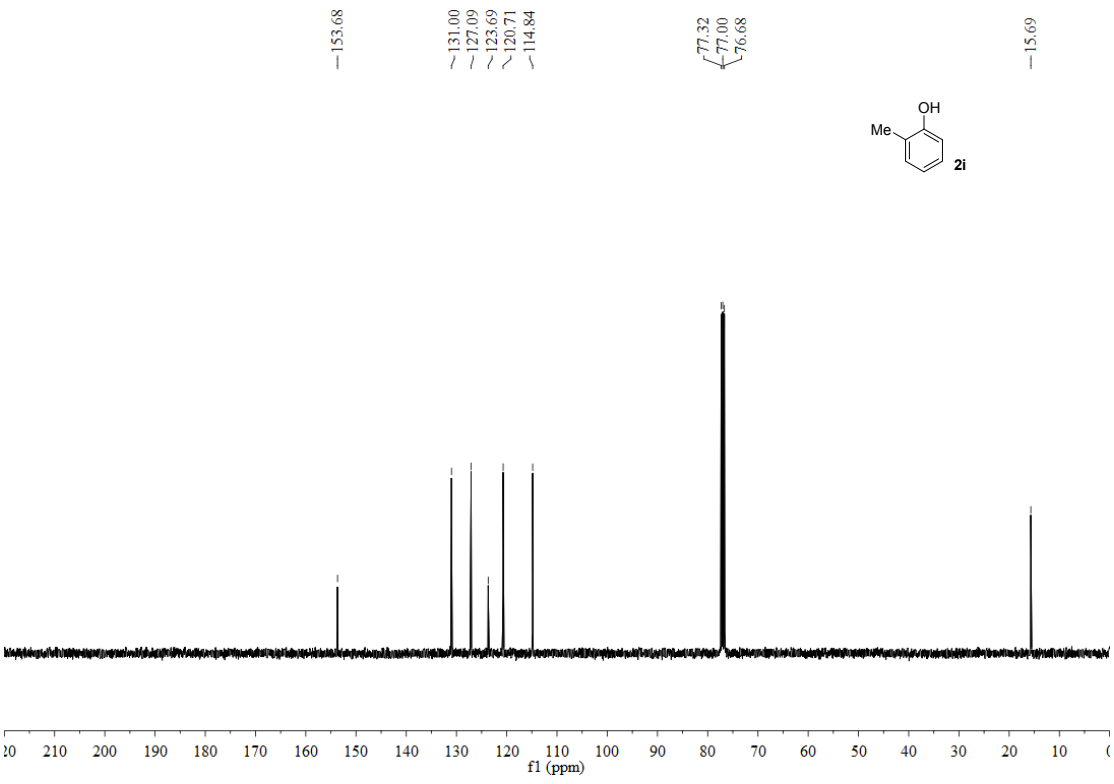
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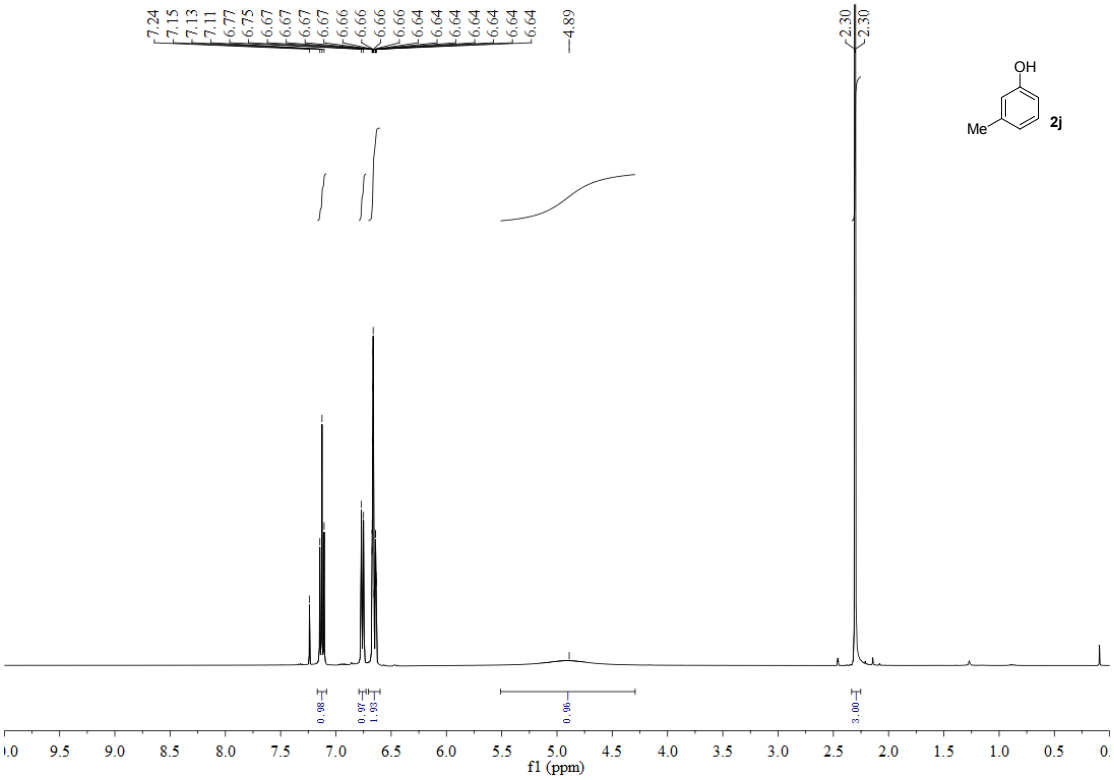
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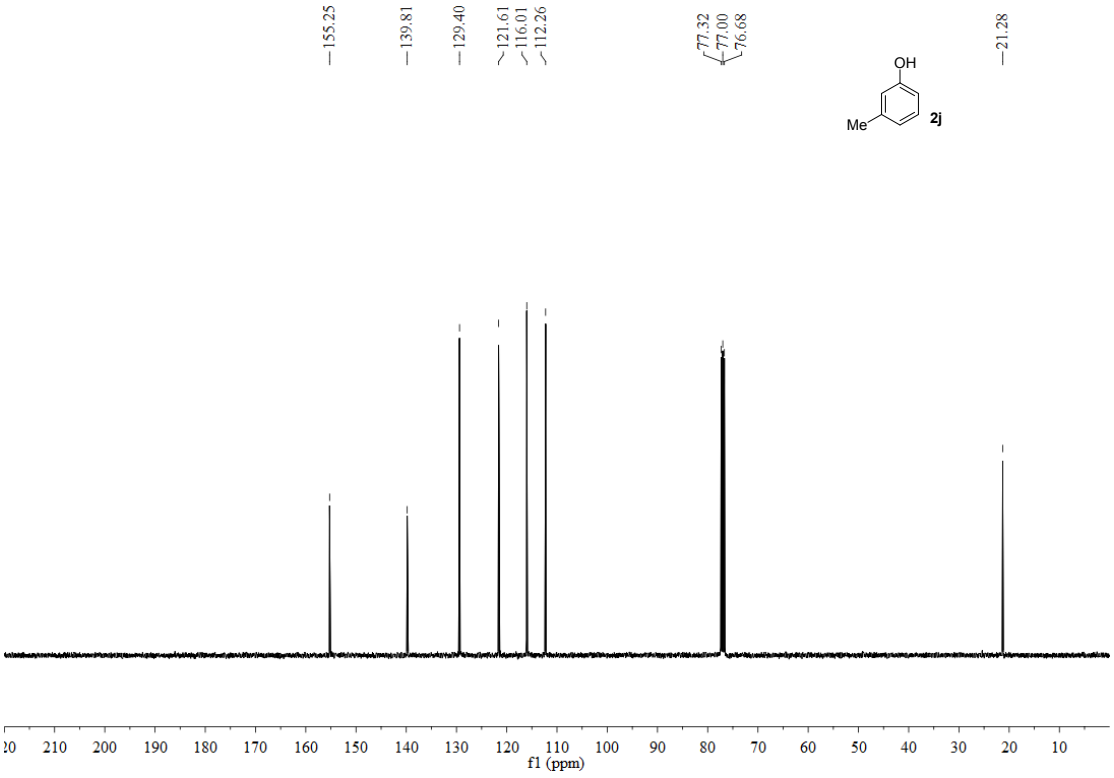
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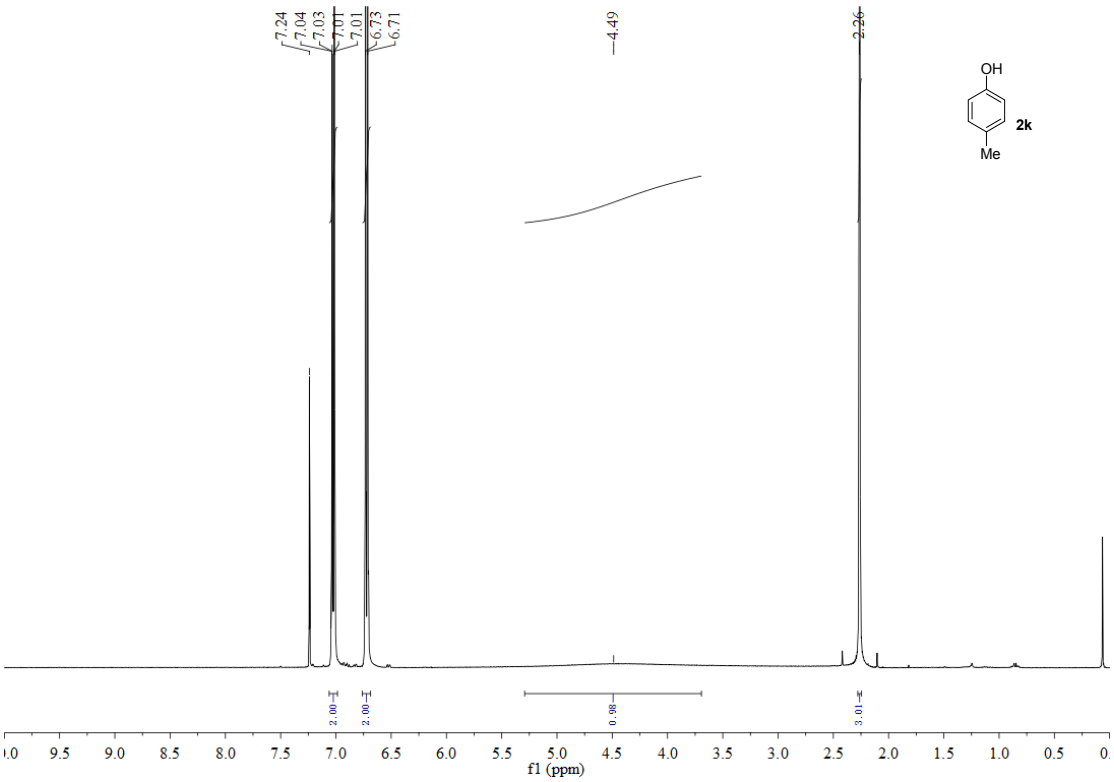
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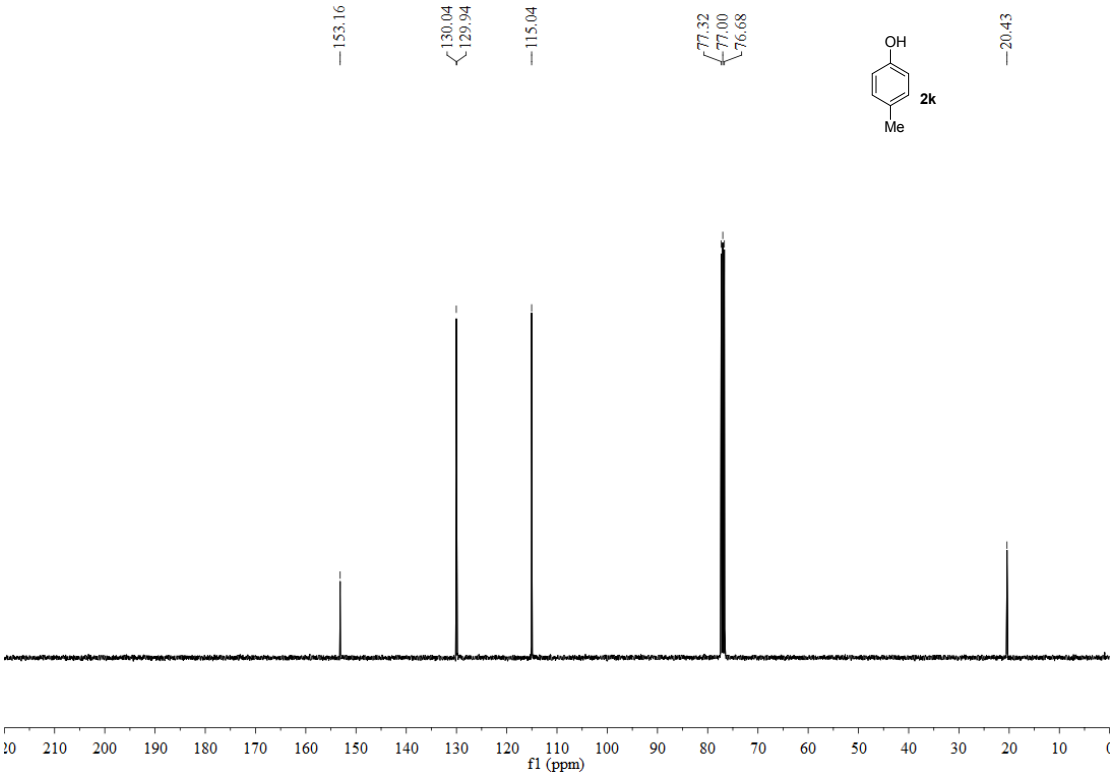
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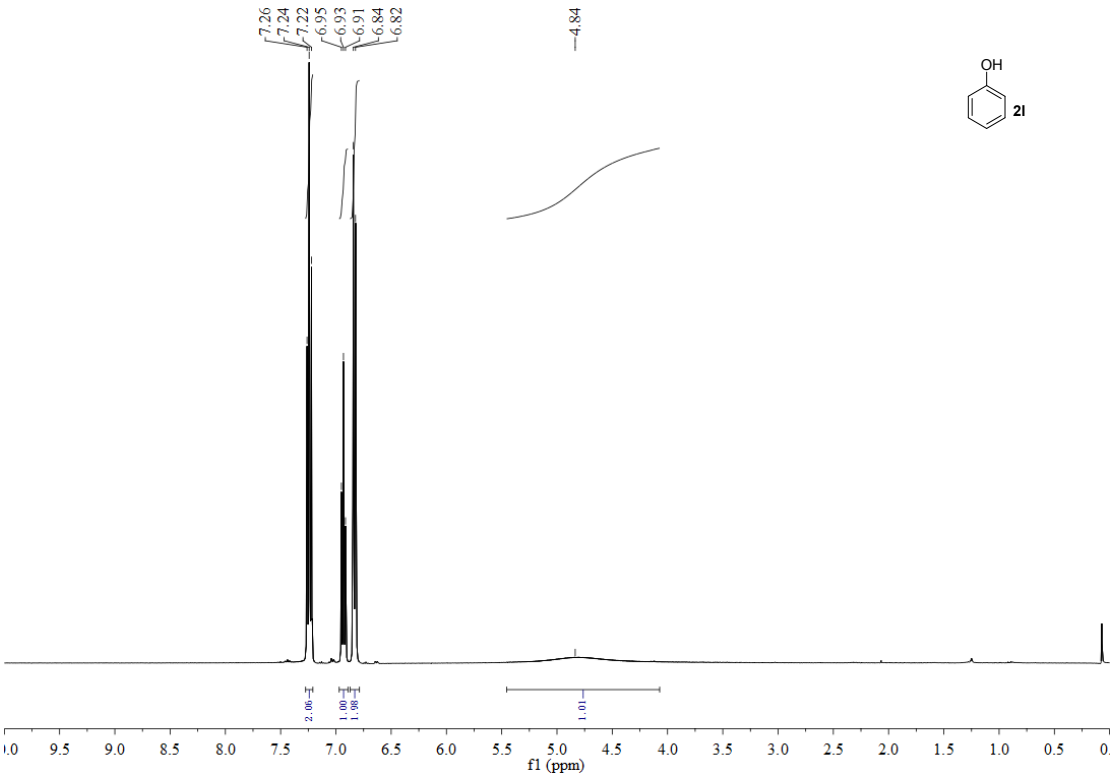
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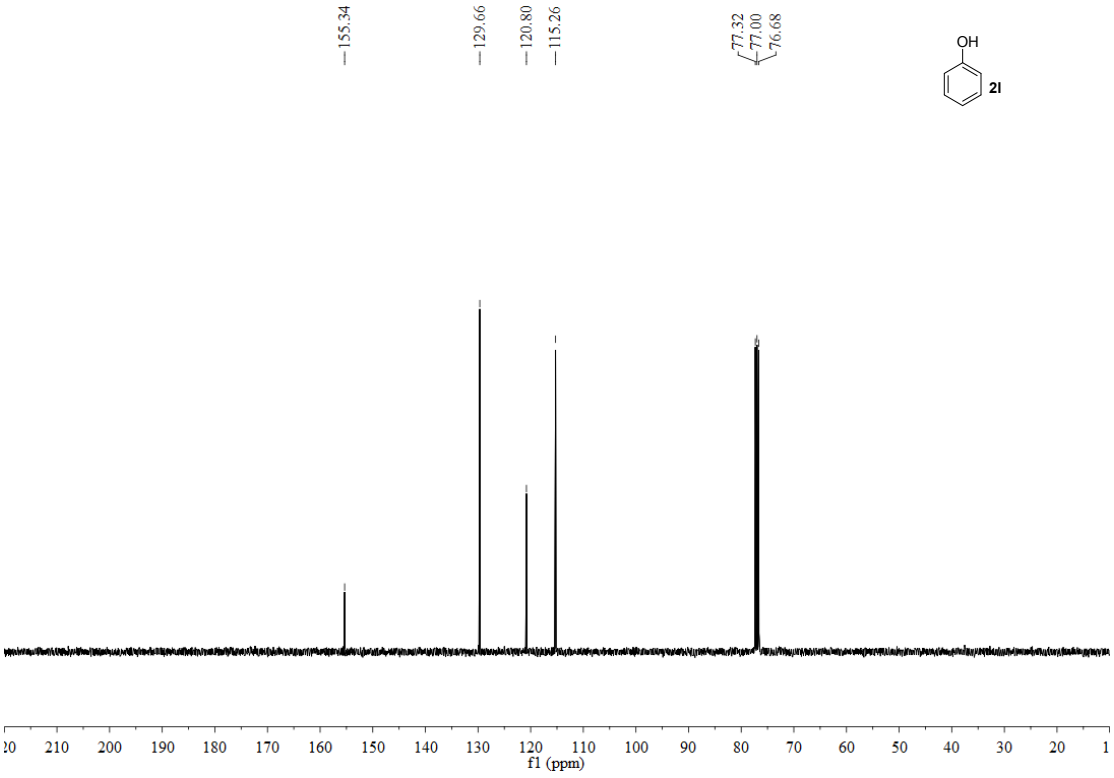
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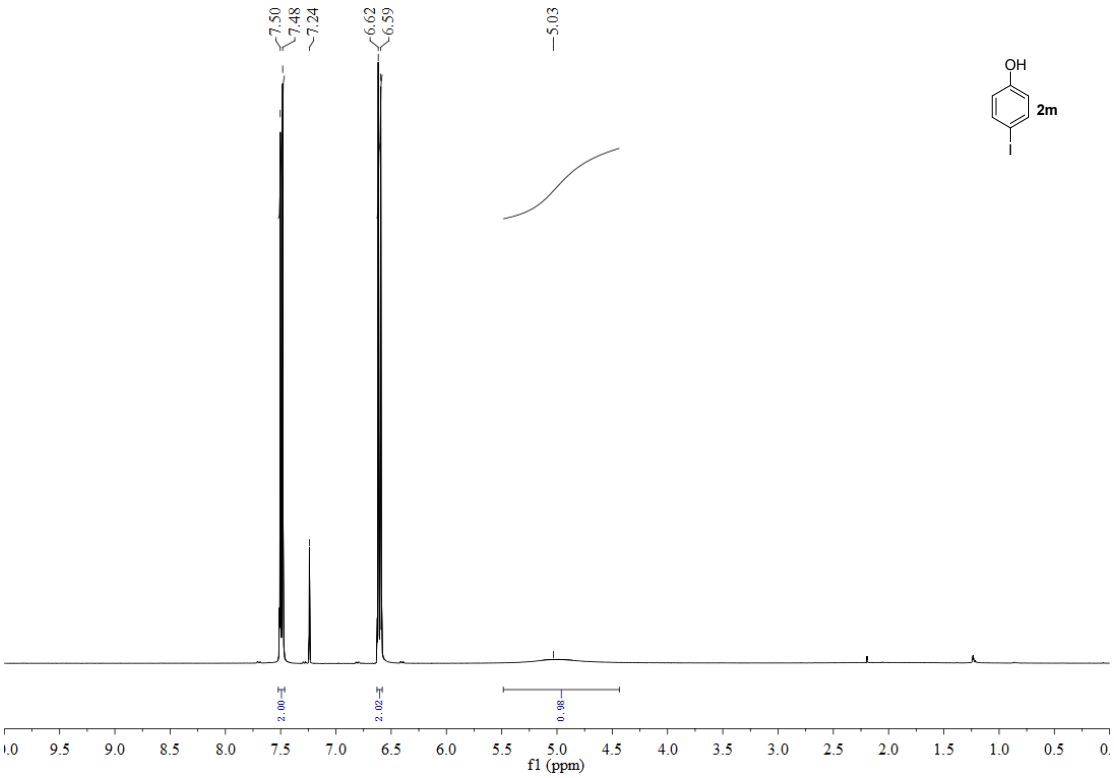
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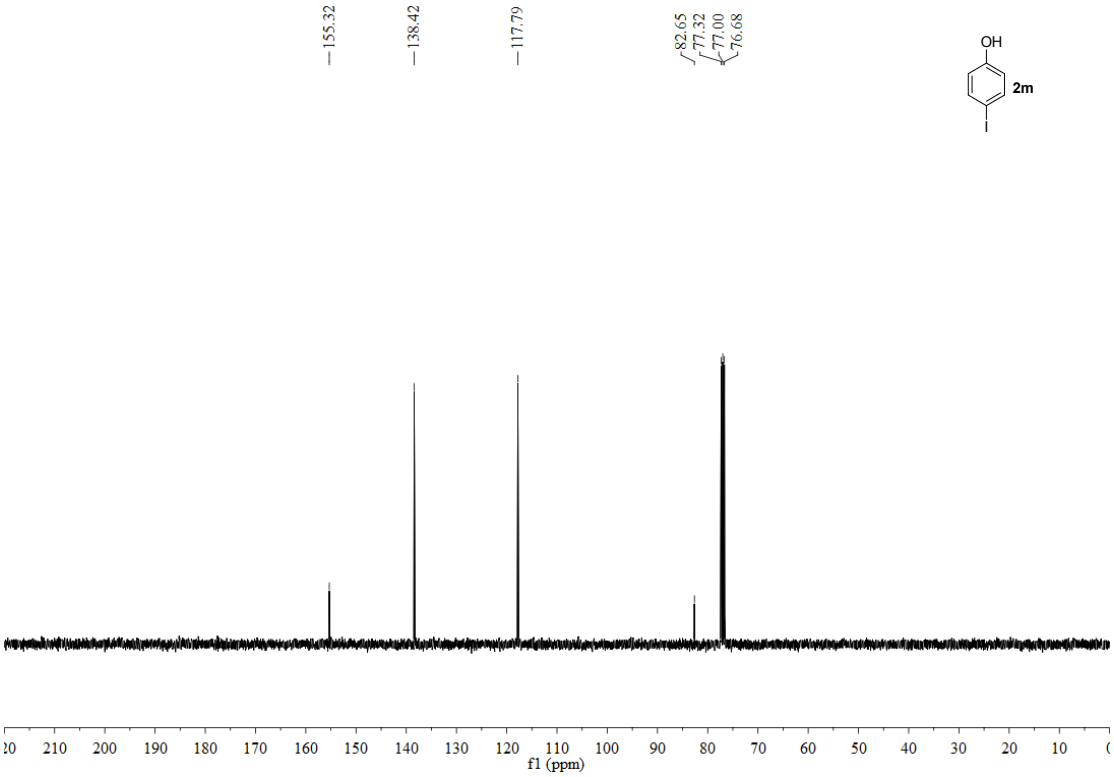
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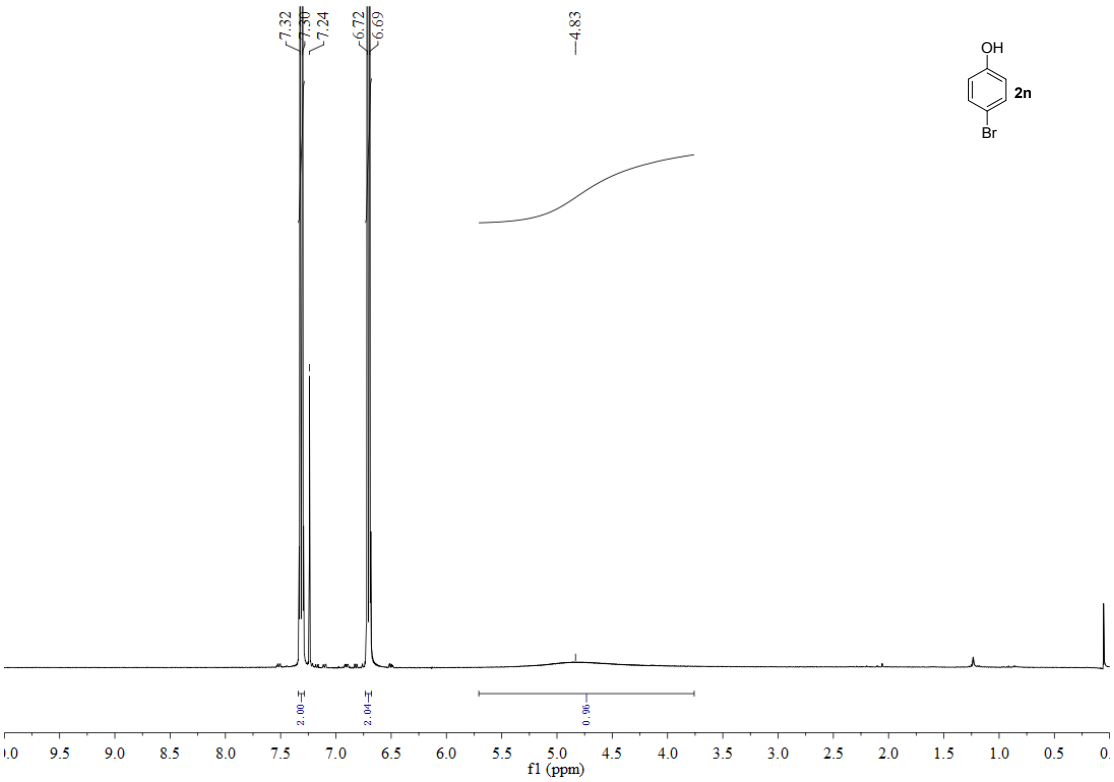
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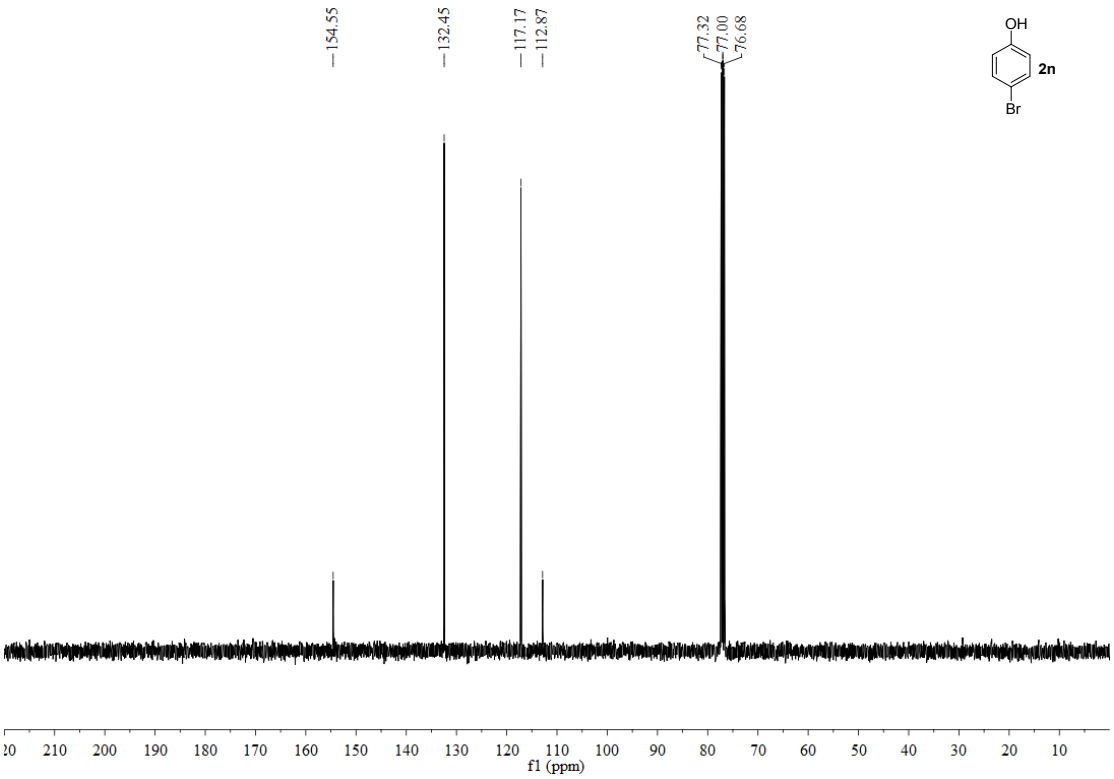
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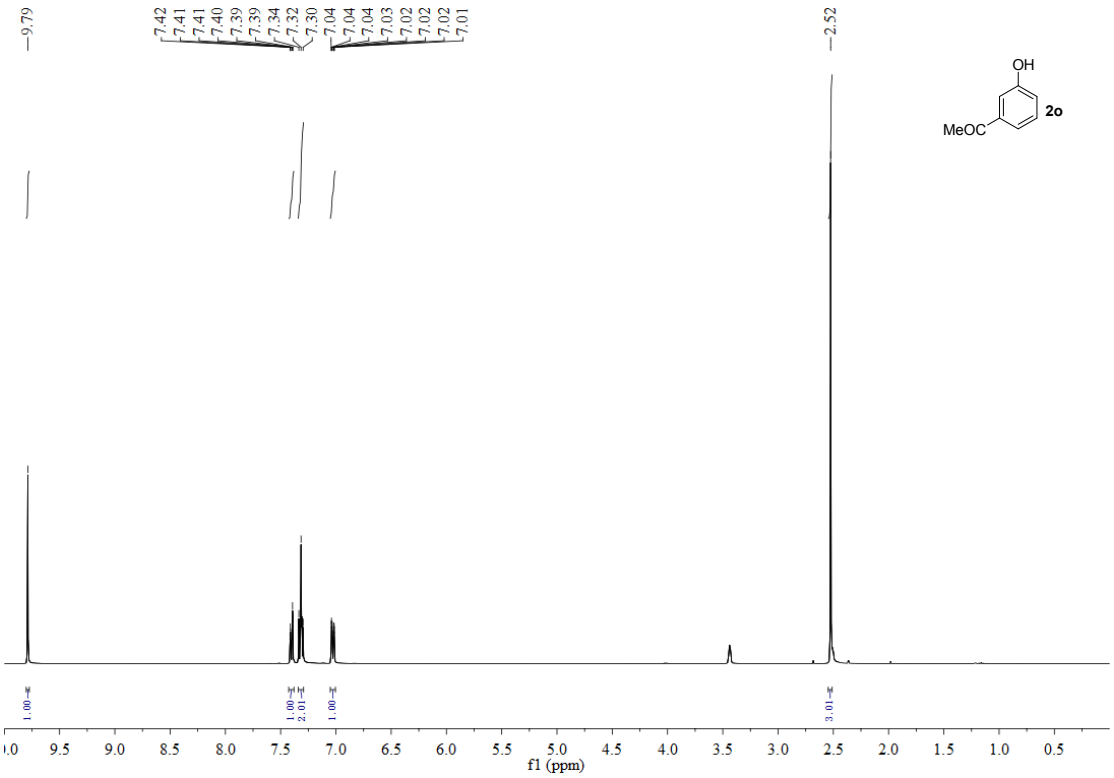
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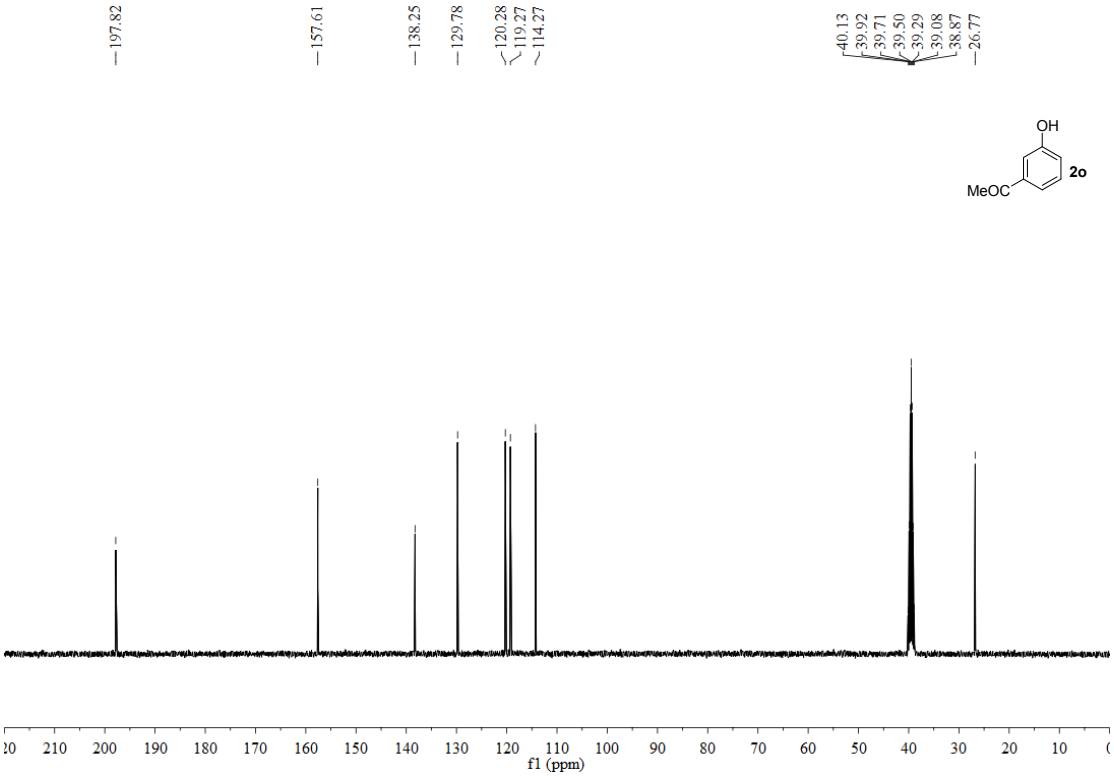
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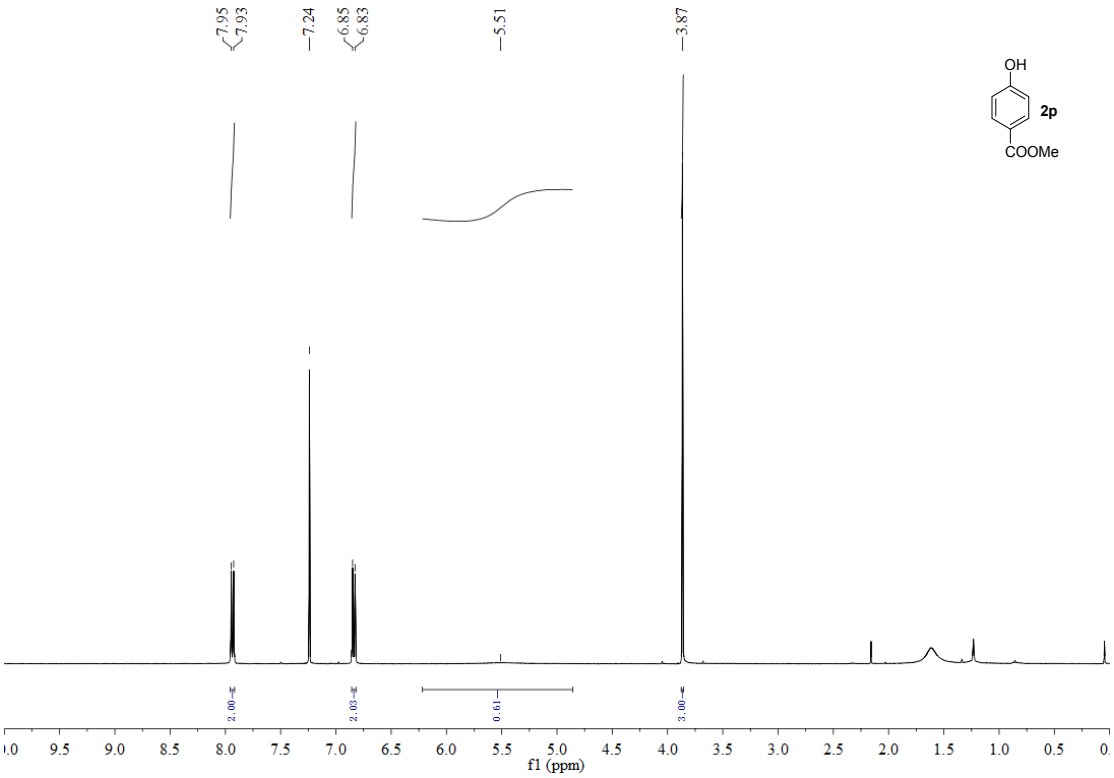
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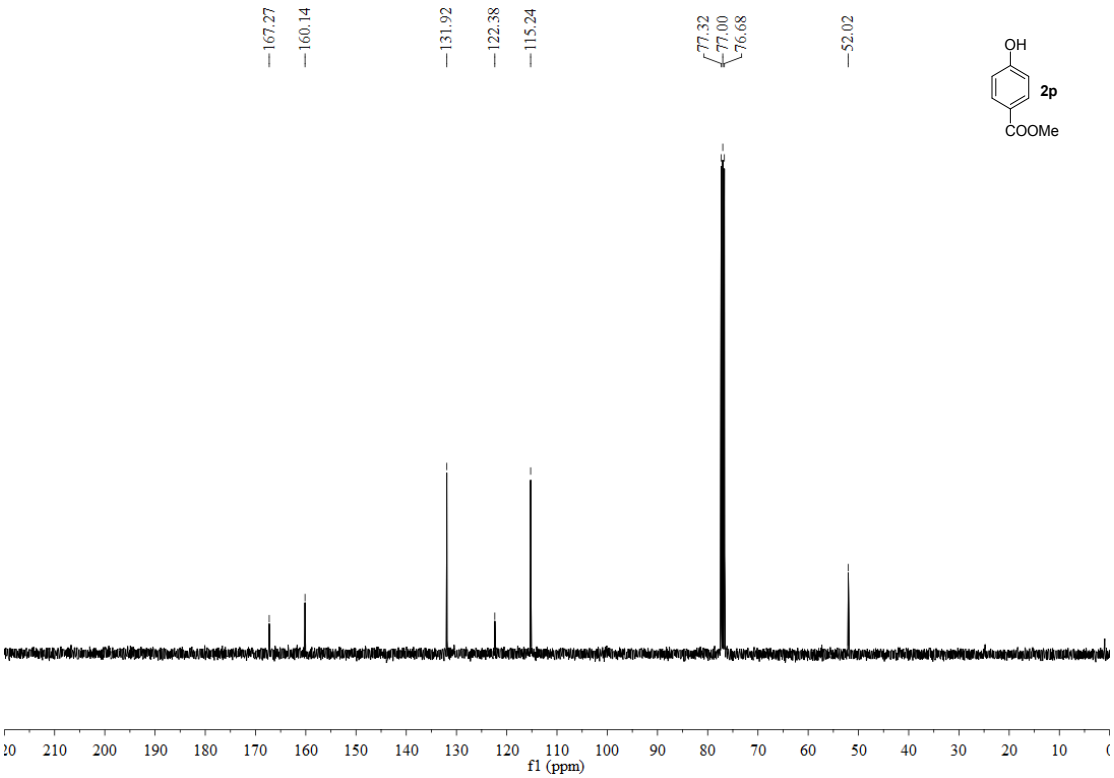
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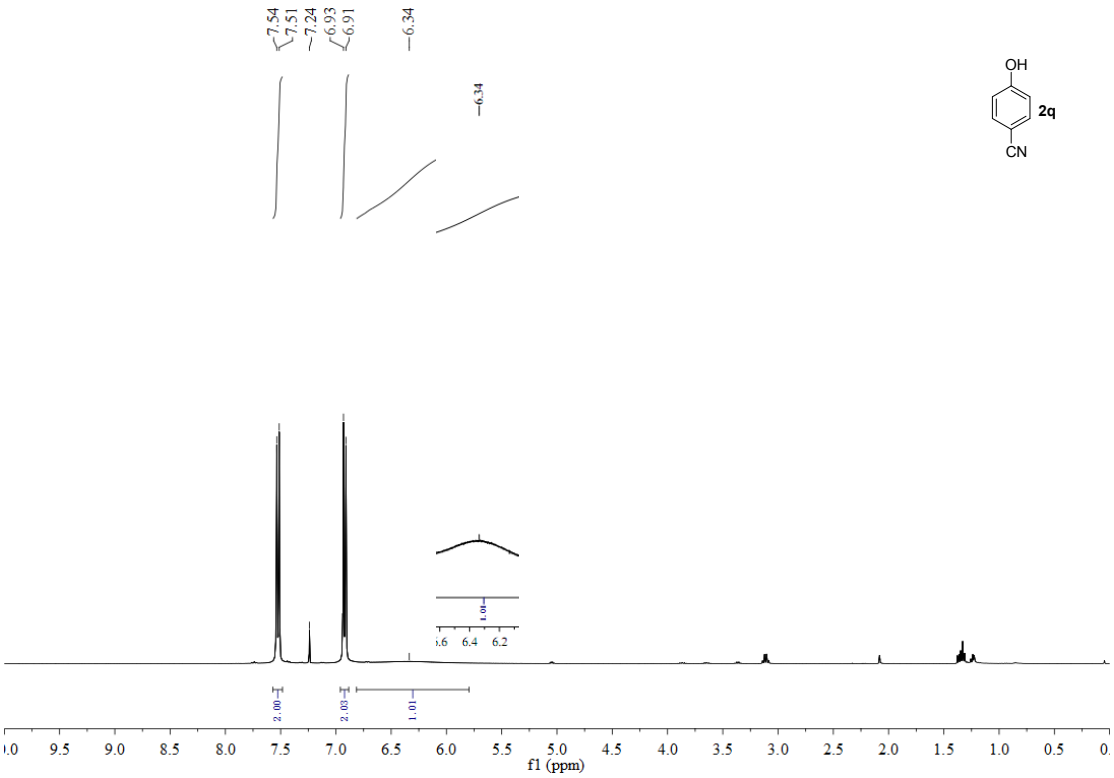
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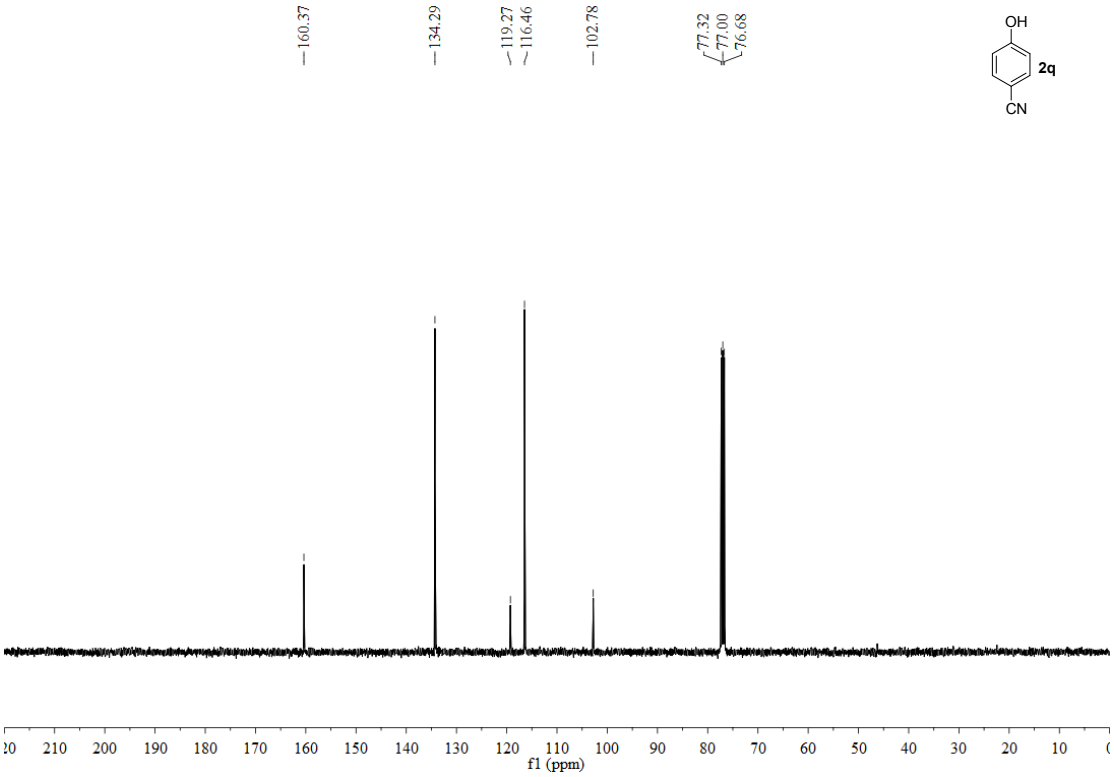
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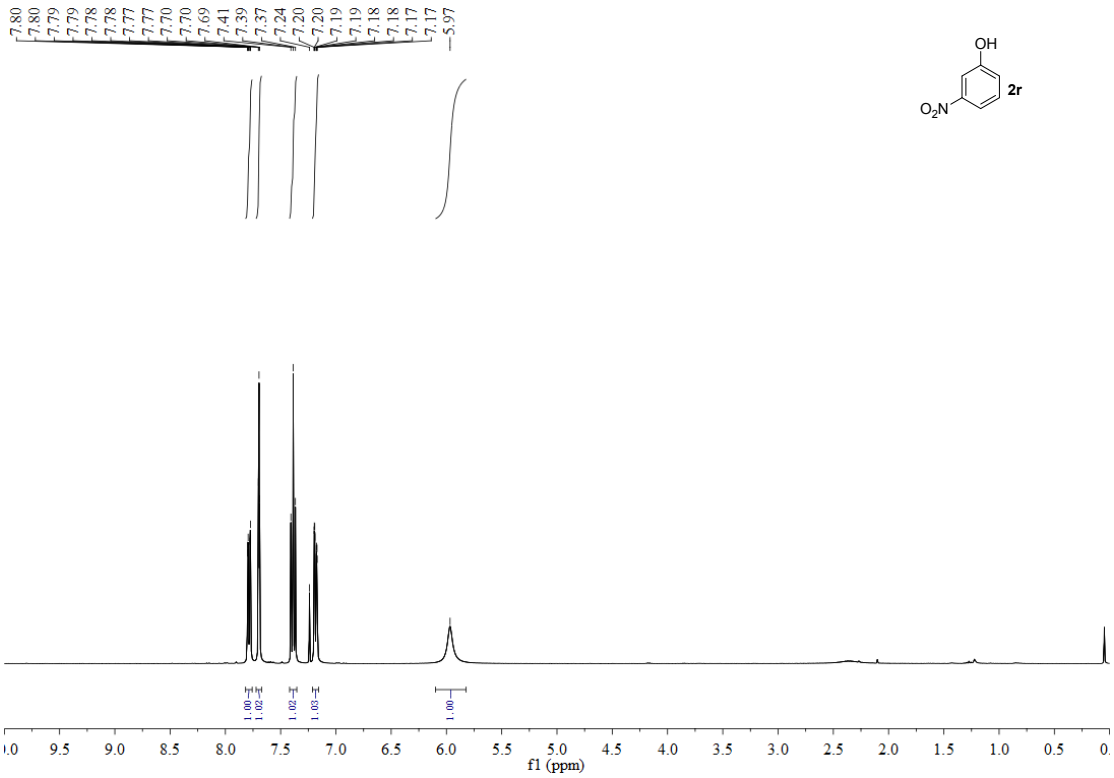
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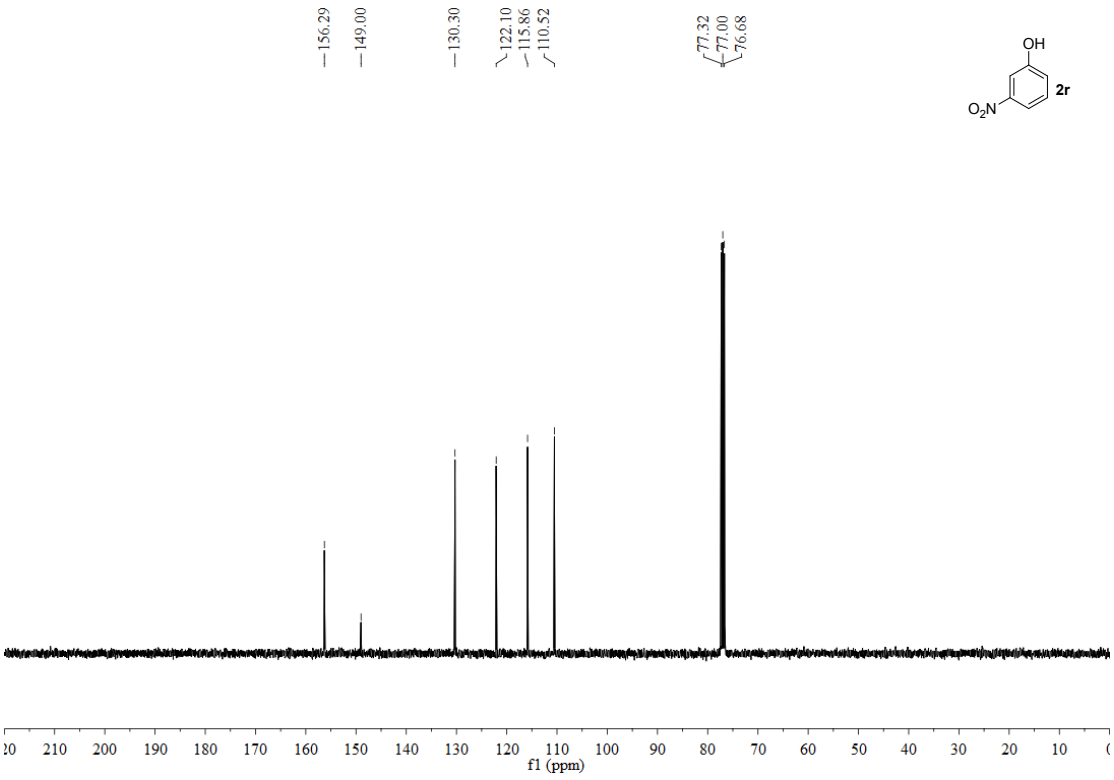
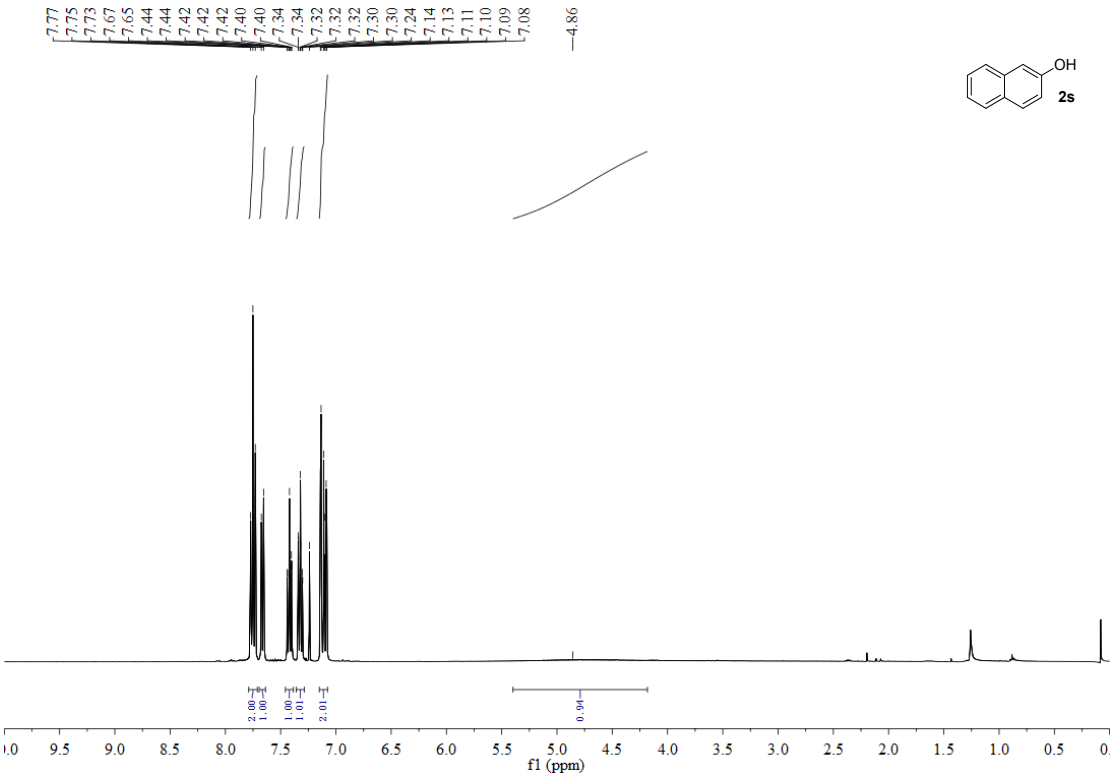
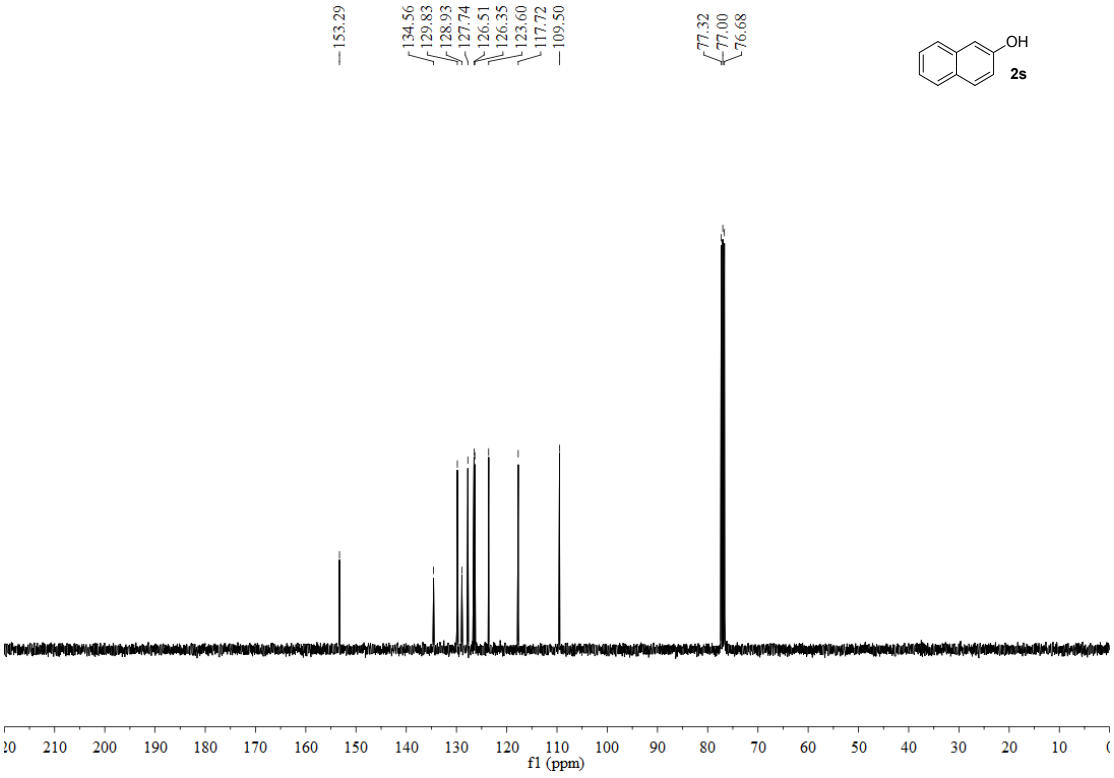
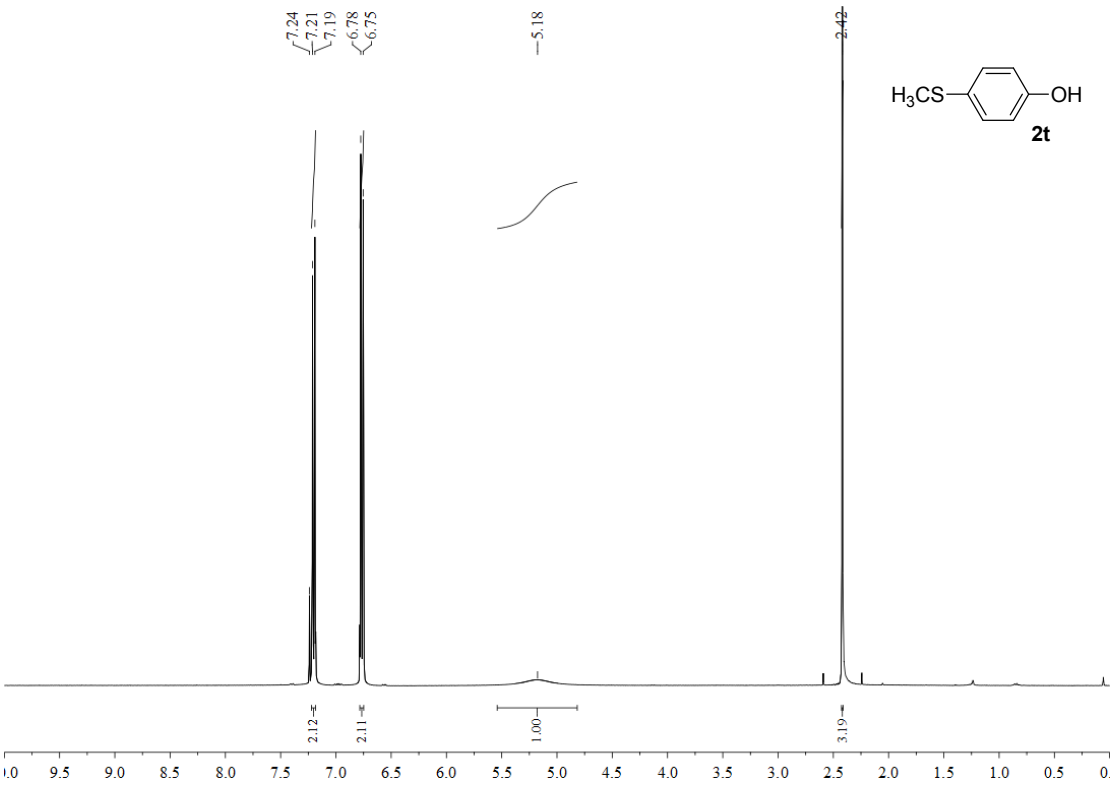
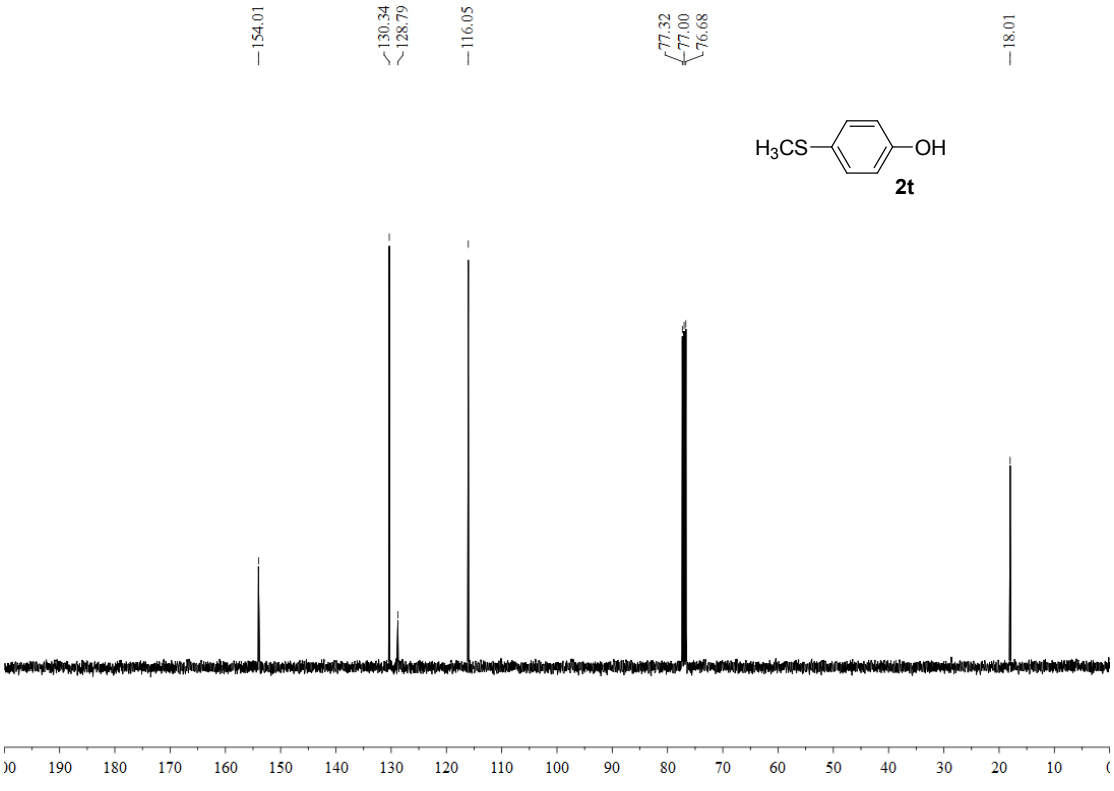
1.00
f1 (ppm)

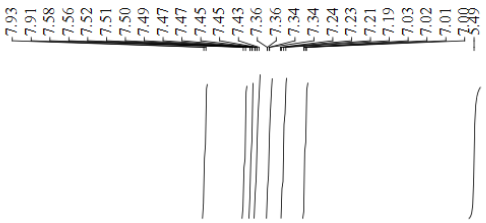

156.29
149.00
130.30
122.10
115.86
110.52
77.32
77.00
76.68
OH
2r
O2N
f1 (ppm)

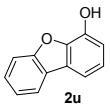

7.77
7.75
7.73
7.67
7.65
7.44
7.44
7.42
7.42
7.42
7.40
7.40
7.34
7.34
7.32
7.32
7.32
7.30
7.30
7.24
7.14
7.13
7.11
7.10
7.09
7.08
4.86
OH
2s
2.00
1.00
1.00
1.01
2.01
0.94
f1 (ppm)


153.29
134.56
129.83
128.93
127.74
126.51
126.35
123.60
117.72
109.50
77.32
77.00
76.68
OH
2s
f1 (ppm)

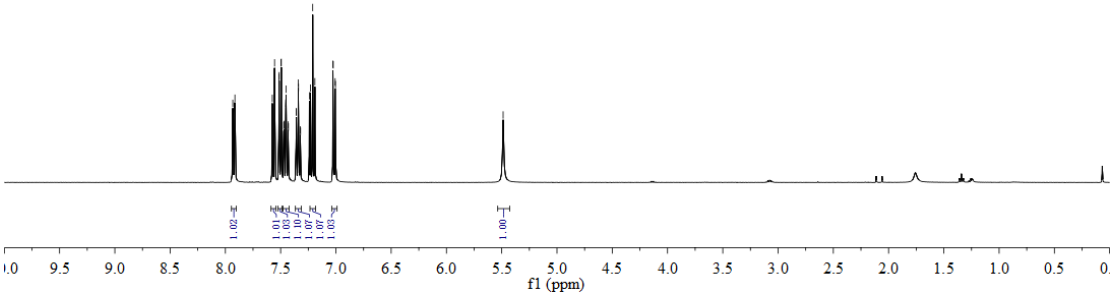

7.24
7.21
7.19
6.78
6.75
5.18
2.42
H3CS
OH
2t
2.12
2.11
1.00
3.19

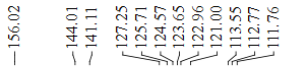

154.01
130.34
128.79
116.05
77.32
77.00
76.68
18.01
H3CS
OH
2t

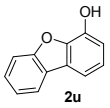

7.93
7.91
7.58
7.56
7.52
7.51
7.50
7.49
7.47
7.47
7.45
7.45
7.43
7.36
7.36
7.34
7.34
7.24
7.23
7.21
7.19
7.03
7.02
7.01
5.49


OH
O

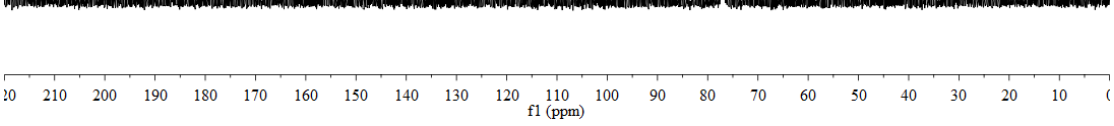
2u

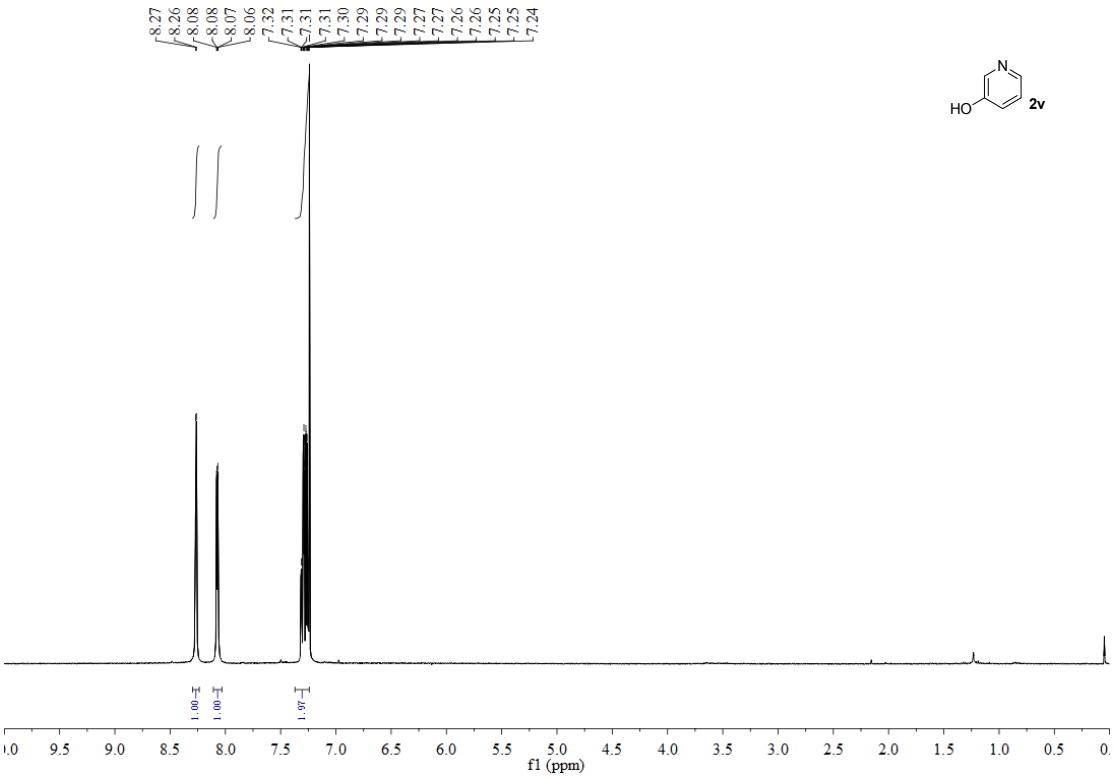

1.02
1.01
1.03
1.10
1.07
1.07
1.03
1.00
f1 (ppm)

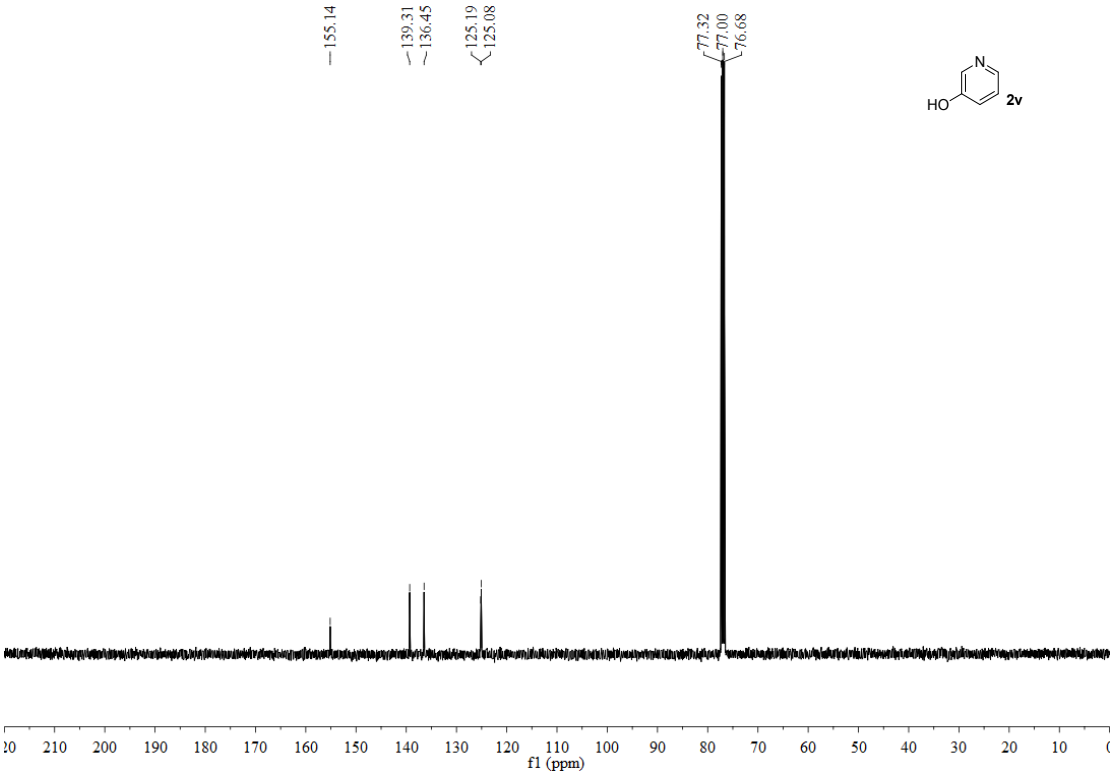

156.02
144.01
141.11
127.25
125.71
124.57
123.65
122.96
121.00
113.55
112.77
111.76
77.32
77.00
76.68

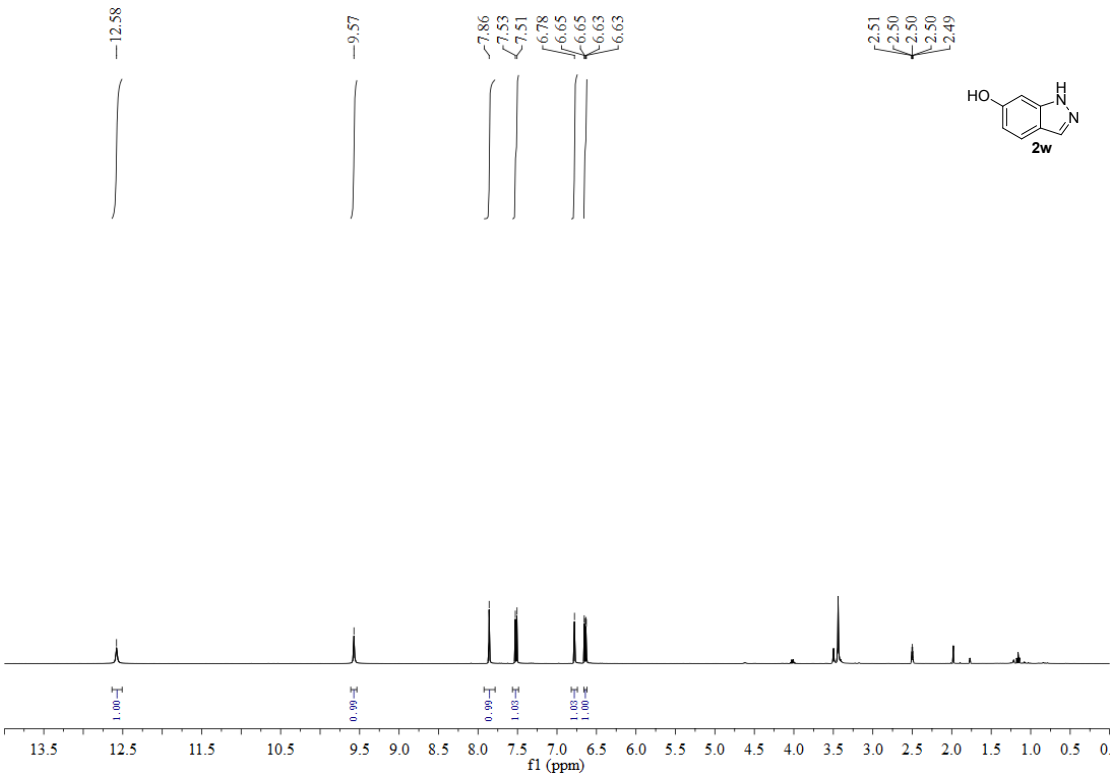

OH
O

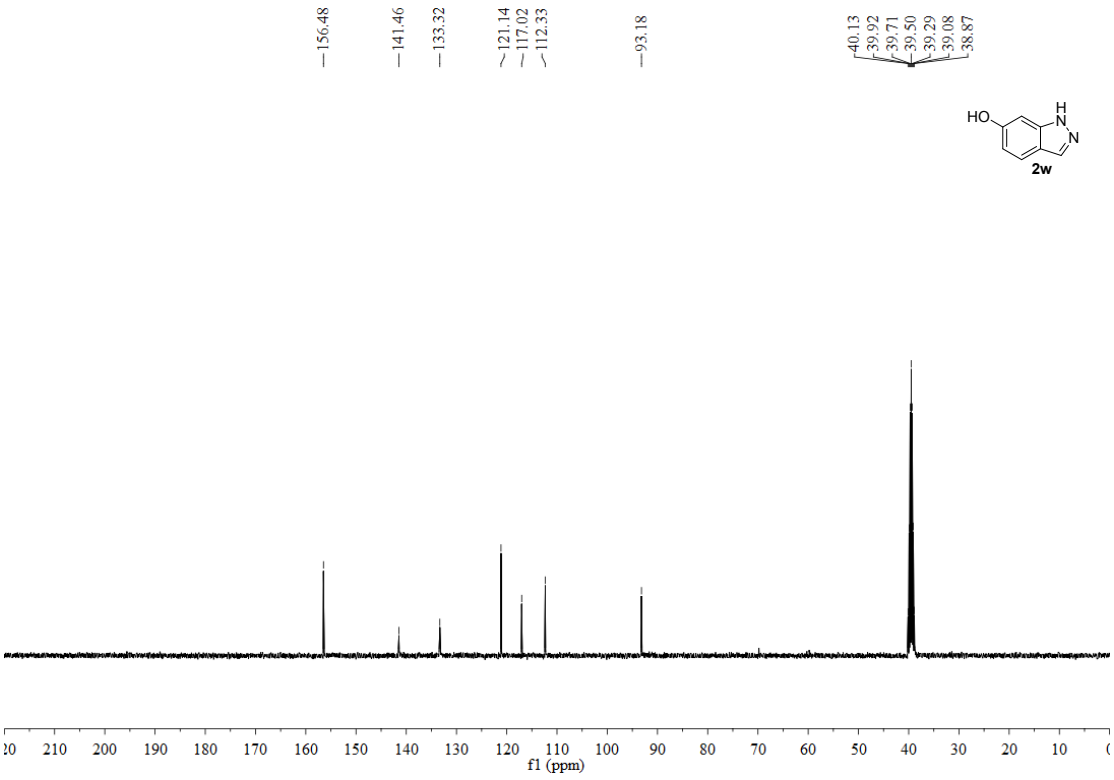
2u


f1 (ppm)


8.27
8.26
8.08
8.08
8.07
8.06
7.32
7.31
7.31
7.31
7.30
7.29
7.29
7.29
7.27
7.27
7.26
7.26
7.25
7.25
7.24
HO
N
2v
1.00
1.00
1.97
f1 (ppm)


155.14
139.31
136.45
125.19
125.08
77.32
77.00
76.68
HO
N
2v
f1 (ppm)


12.58
9.57
7.86
7.53
7.51
6.78
6.65
6.65
6.63
6.63
2.51
2.50
2.50
2.50
2.49
HO
H
N
N
2w
1.00
0.99
0.99
1.03
1.03
1.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


156.48
141.46
133.32
121.14
117.02
112.33
93.18
40.13
39.92
39.71
39.50
39.29
39.08
38.87
HO
H
N
N
2w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)