Supporting information for

Iodine-promoted 2-arylsulfanylphenol formation using cyclohexanones as phenol source

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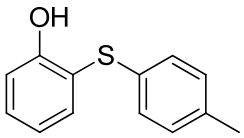
General information

Flash column chromatography was performed over silica gel 48-75 μm. Unless otherwise noted, 1H NMR and 13C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to $SiMe_4$ or chloroform signals. MS analyses were performed on Agilent 5975 GC-MS instrument (EI). The new compounds were characterized by 1H NMR, 13C NMR, MS and HRMS. The structure of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Reagents were used as received or prepared by our laboratory.

General procedure for 3aa:

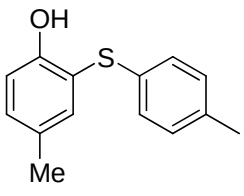
The reaction mixture of cyclohexanone (**1a**, 52 μL, 0.5 mmol), *p*-toluenesulfonyl chloride (**2a**, 114 mg, 0.6 mmol), iodine (25.4 mg, 0.1 mmol) and 1,4-dioxane (1 mL) in a 10 mL oven-dried reaction vessel was stirred at 150 ^{o}C for 18 h under an air atmosphere. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 95:5) to yield the desired product **3aa** as pale yellow liquid (88.6 mg, 82% yield).

2-(*p*-Tolylthio)phenol (3aa, CAS: 59010-83-2):[1]



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.06-7.00 (m, 5H), 6.93 (t, *J* = 6.0 Hz, 1H), 6.53 (s, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.1, 136.7, 136.3, 132.2, 132.1, 130.0, 127.5, 121.2, 117.2, 115.5, 21.0; MS (EI) m/z (%) 216 (100), 201, 183, 96, 91.

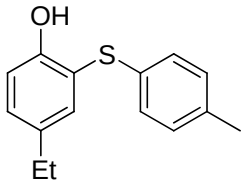
4-Methyl-2-(*p*-tolylthio)phenol (3ba):[1]



Pale yellow liquid; yield 80%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.33 (s, 1H), 7.16 (d, *J* = 8.0

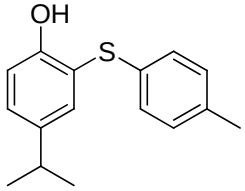
Hz, 1H), 7.06-7.01 (m, 4H), 6.95 (d, J = 8.0 Hz, 1H), 6.36 (s, 1H), 2.28 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.0, 136.7, 136.2, 132.8, 132.5, 130.5, 130.1, 127.6, 116.8, 115.3, 21.0, 20.4; MS (EI) m/z (%) 230 (100), 197, 110, 91, 77, 65.

4-Ethyl-2-(*p*-tolylthio)phenol (3ca):[1]



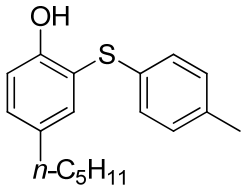
Pale yellow liquid; yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.35 (s, 1H), 7.19 (d, J = 8.0 Hz, 1H), 7.06-6.97 (m, 5H), 6.36 (s, 1H), 2.58 (q, J = 8.0 Hz, 2H) 2.28 (s, 3H), 1.21 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.2, 137.1, 136.2, 135.6, 132.5, 131.6, 130.0, 127.5, 116.8, 115.4, 27.9, 21.0, 15.8; MS (EI) m/z (%) 244 (100), 229, 211, 124, 91, 77.

4-(*iso*-Propyl)-2-(*p*-tolylthio)phenol (3da):



Pale yellow liquid; yield 72%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37 (s, 1H), 7.22 (d, J = 8.0 Hz, 1H), 7.06-6.97 (m, 5H), 6.35 (s, 1H), 2.88-2.82 (m, 1H) 2.28 (s, 3H), 1.22 (d, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.2, 141.8, 136.1, 134.4, 132.5, 130.3, 130.1, 127.3, 116.5, 115.3, 33.3, 24.2, 21.0; MS (EI) m/z (%) 258, 243 (100), 151, 123, 91, 79; HRMS calcd. for: $C_{16}H_{17}OS$ $[M-H]^-$: 257.0995, found 257.0999.

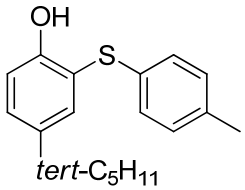
4-Pentyl-2-(*p*-tolylthio)phenol (3ea):[1]



Pale yellow liquid; yield 78%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32 (s, 1H), 7.16 (d, J = 8.0 Hz, 1H), 7.06-6.96 (m, 5H), 6.36 (s, 1H), 2.53 (t, J = 8.0 Hz, 2H), 2.28 (s, 3H), 1.61-1.57 (m, 2H),

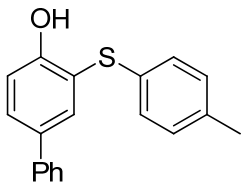
1.33-1.27 (m, 4H), 0.88 (t, J = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.2, 136.2, 136.1, 135.8, 132.6, 132.1, 130.0, 127.4, 116.6, 115.3, 34.9, 31.4, 31.3, 22.6, 21.0, 14.0; MS (EI) m/z (%) 286, 229 (100), 137, 91, 77, 65.

4-(*tert*-Pentyl)-2-(*p*-tolylthio)phenol (3fa):[1]



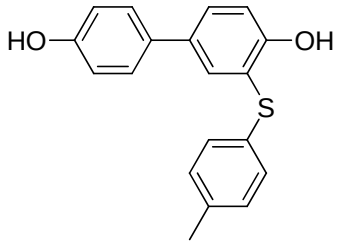
Pale yellow liquid; yield 78%; ^{1}H NMR (400 MHz, CDCl3, ppm) δ 7.46 (s, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.05 (d, J = 8.0 Hz, 2H), 6.98 (t, J = 8.0 Hz, 3H), 6.34 (s, 1H), 2.28 (s, 3H), 1.63-1.59 (m, 2H), 1.25 (s, 6H), 0.67 (t, J = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.8, 142.4, 136.0, 134.3, 132.6, 130.0, 129.9, 126.9, 115.9, 114.9, 37.5, 37.0, 28.6, 20.9, 9.2; MS (EI) m/z (%) 286, 257 (100), 134, 91, 77, 65.

3-(*p*-Tolylthio)-[1,1'-biphenyl]-4-ol (3ga):[1]



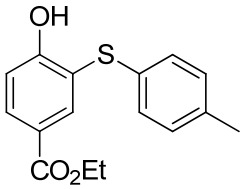
Pale yellow solid; yield 87%; mp 56-58 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.78 (s, 1H), 7.61-7.53 (m, 3H), 7.41 (d, J = 8.0 Hz, 2H), 7.31 (t, J = 8.0 Hz, 1H), 7.14-7.06 (m, 5H), 6.55 (s, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.7, 140.0, 136.5, 135.1, 134.6, 132.2, 130.8, 130.2, 129.0, 127.8, 127.2, 126.8, 118.,0 116.0, 21.1; MS (EI) m/z (%) 292 (100), 172, 139, 91, 77, 65.

3-(*p*-Tolylthio)-[1,1'-biphenyl]-4,4'-diol (3ha):



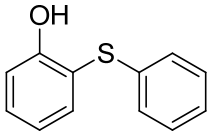
White solid; yield 84%; mp 119-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.71-7.70 (m, 1H), 7.54-7.52 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.11-7.06 (m, 5H), 6.87 (d, *J* = 8.0 Hz, 2H), 6.50 (s, 1H), 4.81 (s, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 157.0, 155.5, 136.8, 132.8, 132.0, 131.0, 130.8, 130.4, 130.2, 127.5, 127.1, 121.5, 116.5, 116.2, 21.1; MS (EI) m/z (%) 308(100), 281, 207, 188, 91, 28; HRMS calcd. for: $C_{19}H_{15}O_2S$ $[M-H]^-$: 307.0787, found 307.0791.

Ethyl 4-hydroxy-3-(*p*-tolylthio)benzoate (3ia):[1]



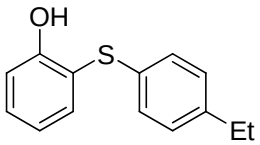
Pale yellow solid; yield 75%; mp 72-74 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.27 (s, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.09-7.03 (m, 5H), 6.95 (s, 1H), 4.34 (q, *J* = 6.7 Hz, 2H), 2.29 (s, 3H), 1.38 (t, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.7, 160.8, 138.4, 136.8, 133.5, 131.3, 130.2, 128.1, 123.7, 118.2, 115.4, 61.0, 21.0, 14.4; MS (EI) m/z (%) 288 (100), 260, 243, 171, 91, 63.

2-(Phenylthio)phenol (3ab, CAS: 55214-86-3):[2]



Pale yellow liquid; yield 65%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.24-7.22 (m, 2H), 7.17-7.13 (m, 1H), 7.09-7.07 (m, 3H) 6.96 (t, *J* = 8.0 Hz, 1H), 6.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.3, 136.9, 135.9, 132.3, 129.2, 127.0, 126.2, 121.3, 116.5, 115.6; MS (EI) m/z (%) 202 (100), 169, 141, 96, 77, 51.

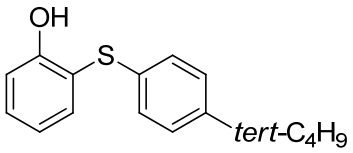
2-((4-Ethyl*phen*yl)thio)phenol (3ac):



Pale yellow liquid; yield 83%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.36

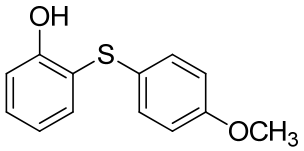
(t, *J* = 8.0 Hz, 1H), 7.08-7.02 (m, 5H), 6.94 (t, *J* = 8.0 Hz, 1H), 6.55 (s, 1H); 2.61-2.55 (m, 2H),1.18 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.2, 142.7, 136.7, 132.4, 132.0, 128.8, 127.6, 121.1, 117.3, 115.5, 28.3, 15.4; MS (EI) m/z (%) 230 (100), 215, 105, 91, 77, 63; HRMS calcd. for: $C_{14}H_{13}OS$ $[M-H]^-$: 229.0682, found 229.0686.

2-((4-(*tert*-Butyl)phenyl)thio)phenol (3ad, CAS: 2976-28-5):[3]



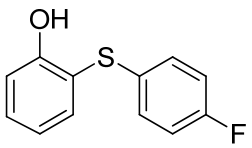
Pale yellow liquid; yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.28-7.26 (m, 2H), 7.08-7.03 (m, 3H), 6.95 (t, *J* = 8.0 Hz, 1H), 6.55 (s, 1H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.3, 149.5, 136.9, 132.3, 132.2, 127.0, 126.4, 121.3, 116.9, 115.6, 34.5, 31.3; MS (EI) m/z (%) 258, 243(100), 125, 108, 97, 77.

2-((4-Methoxyphenyl)thio)phenol (3ae):[1]



Pale yellow solid; yield 64%; mp 62-64 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) *δ* 7.50 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.91 (t, *J* = 8.0 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.57 (s, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) *δ* 159.0, 156.8, 136.1, 131.6, 130.3, 126.2, 121.2, 118.8, 115.5, 115.1, 55.4; MS (EI) *m/z* (%) 232 (100), 217, 171, 108, 96.

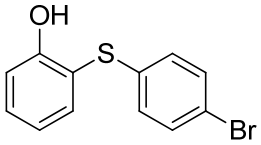
2-((4-Fluorophenyl)thio)phenol (3af):[1]



Pale yellow liquid; yield 80%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) *δ* 7.51 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.11-7.06 (m, 3H), 6.97-6.93 (m, 3H), 6.49 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) *δ* 161.7 (d, *J* = 243.0 Hz), 157.1, 136.6, 132.3, 130.9 (d, *J* = 3.0 Hz), 129.3 (d, *J* =

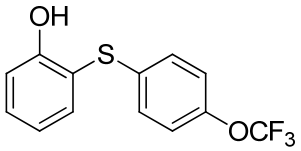
8.0 Hz), 121.4, 117.1, 116.4 (d, J = 22.0 Hz), 115.7; MS (EI) *m/z* (%) 220, 128, 96 (100), 75, 61.

2-((4-Bromophenyl)thio)phenol (3ag, CAS: 1254831-59-8):[1]



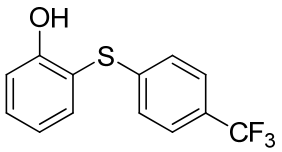
Pale yellow liquid; yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.51 (d, J = 8.0 Hz, 1H), 7.42-7.34 (m, 3H), 7.08 (d, J = 8.0 Hz, 1H), 6.99-6.92 (m, 3H), 6.42 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.3, 136.9, 135.2, 132.7, 132.3, 128.4, 121.6, 120.0, 115.8, 115.8; MS (EI) *m/z* (%) 282, 280, 201, 168, 96 (100).

2-((4-(Trifluoromethoxy)phenyl)thio)phenol (3ah):



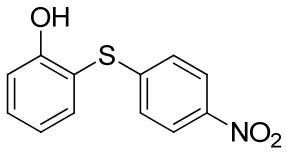
Pale yellow liquid; yield 66%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.53 (d, J = 8.0 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.10-7.08 (m, 5H), 6.98 (d, J = 8.0 Hz, 1H), 6.45 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 157.3, 147.6, 136.9, 134.7, 132.7, 128.0, 121.9, 121.6, 120.4 (q, J = 256.0 Hz), 115.8, 115.7; MS (EI) *m/z* (%) 286 (100), 201, 171, 128, 96; HRMS calcd. for: $C_{13}H_8O_2F_3S$ $[M-H]^-$: 285.0192, found 285.0195.

2-((4-(Trifluoromethyl)phenyl)thio)phenol (3ai):



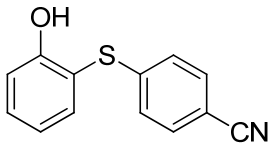
Pale yellow liquid; yield 46%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.53 (d, J = 8.0 Hz, 1H), 7.48-7.43 (m, 3H), 7.12 (d, J = 8.0 Hz, 3H), 7.01 (t, J = 8.0 Hz, 1H), 6.37 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 157.4, 141.2, 137.1, 133.0, 128.1 (q, J = 32.0 Hz), 126.1, 126.0 (q, J = 3.7 Hz), 124.0 (q, J = 270.0 Hz), 121.7, 116.0, 114.5; MS (EI) *m/z* (%) 270 (100), 251, 171, 96, 69; HRMS calcd. for: $C_{13}H_8OF_3S$ $[M-H]^-$: 269.0243, found 269.0247.

2-((4-Nitrophenyl)thio)phenol (3aj):[4]



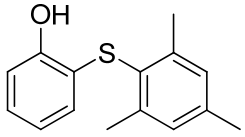
Yellow solid; yield 36%; mp 99-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.09 (d, J = 8.0 Hz, 2H), 7.54-7.46 (m, 2H), 7.15-7.11 (m, 3H), 7.04 (t, J = 8.0 Hz, 1H), , 6.25 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.5, 145.9, 137.1, 133.4, 126.5, 126.0, 124.4, 124.2, 121.9, 116.3; MS (EI) *m/z* (%) 247 (100), 230, 200, 171, 97.

4-((2-Hydroxyphenyl)thio)benzonitrile (3ak):[5]



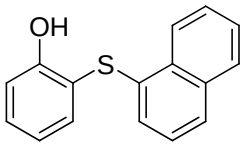
Pale yellow solid; yield 42%; mp 82-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.52-7.44 (m, 4H), 7.13-7.07 (m, 3H), 7.02 (t, J = 8.0 Hz, 1H), , 6.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.5, 143.5, 137.1, 133.3, 132.8, 132.6, 126.7, 126.3, 121.8, 118.5, 116.2; MS (EI) *m/z* (%) 227 (100), 198, 166, 96, 63.

2-(Mesitylthio)phenol (3al):



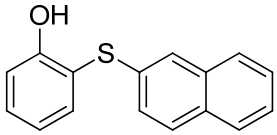
Pale yellow solid; yield 75%; mp 61-63 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.08 (t, J = 8.0 Hz, 1H), 6.96 (s, 2H), 6.90 (d, J = 8.0 Hz, 1H), 6.84 (d, J = 8.0 Hz, 1H), 6.74 (t, J = 6.0 Hz, 1H), 5.84 (s, 1H), 2.39 (s, 6H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.1, 142.9, 139.1, 129.9, 129.7, 127.9, 122.2, 121.4, 115.4, 110.0, 21.9, 21.1; MS (EI) *m/z* (%) 244, 150, 120 (100), 105, 91, 77; HRMS calcd. for: $C_{15}H_{15}OS$ $[M-H]^-$: 243.0838, found 243.0842.

2-(Naphthalen-1-ylthio)phenol (3am):



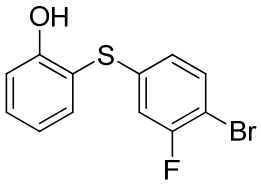
Pale yellow solid; yield 73%; mp 87-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.35 (d, J = 8.0 Hz, 1H), 7.87 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.63-7.54 (m, 3H), 7.41 (t, J = 6.0 Hz, 1H), 7.30-7.28 (m, 1H), 7.11 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 8.0 Hz, 1H), 6.90 (d, J = 8.0 Hz, 1H), 6.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.4, 136.9, 134.1, 133.0, 132.2, 131.4, 128.8, 126.9, 126.7, 126.5, 126.0, 124.6, 124.0, 121.6, 116.3, 115.9; MS (EI) *m/z* (%) 252, 189, 128 (100), 115, 77; HRMS calcd. for: $C_{16}H_{11}OS$ $[M-H]^-$: 251.0525, found 251.0530.

2-(Naphthalen-2-ylthio)phenol (3an):[1]



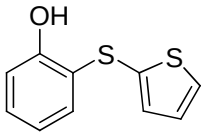
Pale yellow liquid; yield 79%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77-7.58 (m, 4H), 7.48-7.40 (m, 4H), 7.24-7.21 (m, 1H), 7.11 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 8.0 Hz, 1H), 6.54 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.4, 136.9, 133.8, 133.2, 132.3, 131.9, 129.0, 127.8, 127.2, 126.8, 125.9, 125.4, 125.3, 121.4, 116.6, 115.8; MS (EI) *m/z* (%) 252, 219, 128 (100), 115, 77.

2-((4-Bromo-3-fluorophenyl)thio)phenol (3ao):



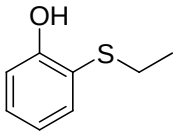
Pale yellow liquid; yield 56%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.51 (d, J = 8.0 Hz, 1H), 7.45-7.38 (m, 2H), 7.10 (d, J = 8.0 Hz, 1H), 7.00 (t, J = 8.0 Hz, 1H), 6.77-6.74 (m, 2H), 6.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 159.4 (d, J = 248.0 Hz), 157.3, 138.0 (d, J = 6.0 Hz), 136.9, 133.9, 133.0, 123.4 (d, J = 4.0 Hz), 121.7, 116.1, 115.0, 114.7 (d, J = 25.0 Hz), 106.4 (d, J = 21.0 Hz); MS (EI) *m/z* (%) 300 (100), 218, 186, 109, 96, 63; HRMS calcd. for: $C_{12}H_7BrFOS$ $[M-H]^-$: 296.9380, found 296.9382.

2-(Thiophen-2-ylthio)phenol (3ap):



Pale yellow solid; yield 43%; mp 39-41 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.52 (d, J = 8.0 Hz, 1H), 7.30-7.29 (m, 2H), 7.15 (s, 1H), 7.00-6.87 (m, 3H), 6.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 156.0, 134.9, 133.6, 132.1, 131.5, 129.1, 127.6, 121.2, 120.4, 115.7; MS (EI) *m/z* (%) 208 (100), 175, 147, 96, 84, 71; HRMS calcd. for: $C_{10}H_7OS_2$ $[M-H]^-$: 206.9933, found 206.9935.

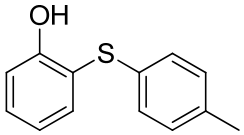
2-(Ethylthio)phenol (3aq, CAS: 29549-60-8)[6]:



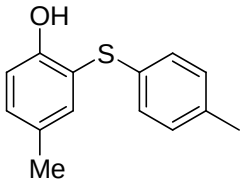
Pale yellow liquid; yield 43%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.47 (d, J = 8.0 Hz, 1H), 7.32-7.26 (m, 1H), 6.99 (d, J = 8.0 Hz, 1H), 6.88 (t, J = 6.0 Hz, 1H), 6.77 (s, 1H), 2.72 (q, J = 8.0 Hz, 2H), 1.22 (t, J = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.1, 136.1, 131.1, 120.7, 118.8, 114.7, 30.8, 14.9; MS (EI) *m/z* (%) 154 (100), 139, 126, 97, 53.

General procedure (5aa):

Iodine (15.3 mg, 0.06 mmol) and *p*-toluenesulfinic acid sodium (**4a**, 107 mg, 0.6 mmol) were added to a 10 mL oven-dried reaction vessel. The reaction vessel was purged with argon for three times and was added diether phosphite (50 μL, 0.4 mmol), cyclohexanone (**1a**, 21 μL, 0.2 mmol), DMSO (0.1 mL) and toluene (0.5 mL) by syringe. The reaction mixture was stirred at 130 ^{o}C for 24 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 98:2) to yield the desired product **5aa** as pale yellow liquid (30.6 mg, 71% yield). The product is same as **3aa**.

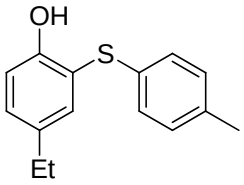


4-Methyl-2-(*p*-tolylthio)phenol (5ba):[1]



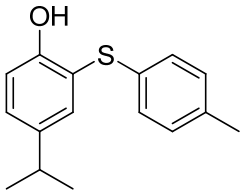
Pale yellow liquid; yield 75%. The product is same as **3ba**.

4-Ethyl-2-(*p*-tolylthio)phenol (5ca):[1]



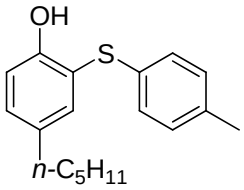
Pale yellow liquid; yield 83%. The product is same as **3ca**.

4-(*iso*-Propyl)-2-(*p*-tolylthio)phenol (5da):



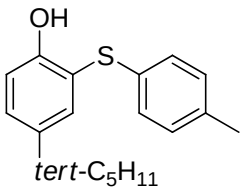
Pale yellow liquid; yield 81%. The product is same as **3da**.

4-Pentyl-2-(*p*-tolylthio)phenol (5ea):[1]



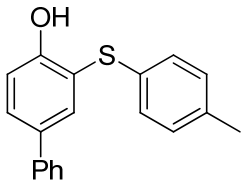
Pale yellow liquid; yield 83%. The product is same as **3ea**.

4-(*tert*-Pentyl)-2-(*p*-tolylthio)phenol (5fa):[1]



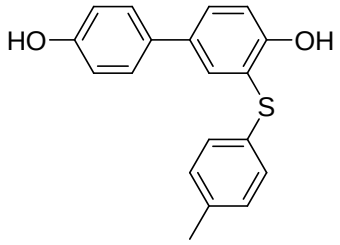
Pale yellow liquid; yield 85%. The product is same as **3fa**.

3-(*p*-Tolylthio)-[1,1'-biphenyl]-4-ol (5ga):[1]



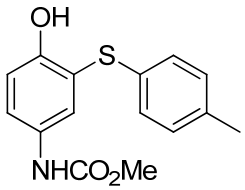
Pale yellow solid; yield 80%. The product is same as **3ga**.

3-(*p*-Tolylthio)-[1,1'-biphenyl]-4,4'-diol (5ha):



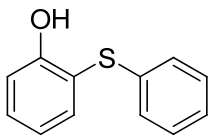
White solid; yield 68%. The product is same as **3ha**.

N-(4-Hydroxy-3-(*p*-tolylthio)phenyl)acetamide (5ia):[1]



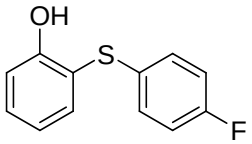
Pale yellow liquid; yield 50%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.62 (s, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.05-6.99 (m, 6H), 6.38 (s, 1H), 2.28 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 168.5, 153.8, 136.6, 131.7, 131.2, 130.1, 128.1, 128.0, 124.5, 117.9, 115.6, 24.2, 21.0; MS (EI) *m/z* (%) 273 (100), 231, 207, 139, 111, 91.

2-(Phenylthio)phenol (5ab, CAS: 55214-86-3):[2]



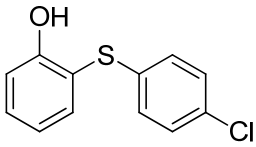
Pale yellow liquid; yield 64%. The product is same as **3ab**.

2-((4-Fluorophenyl)thio)phenol (5ac):[1]



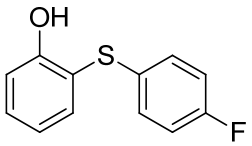
Pale yellow liquid; yield 75%. The product is same as **3af**.

2-((4-Chlorophenyl)thio)phenol (5ad, CAS: 59010-71-8):[1]



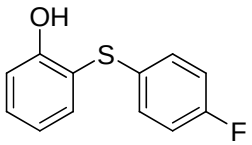
Pale yellow liquid; yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.51 (d, J = 8.0 Hz, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.19 (t, J = 8.0 Hz, 2H), 7.09-6.95 (m, 4H), 6.43 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.2, 136.8, 134.5, 132.5, 132.3, 129.3, 128.3, 121.4, 116.2, 115.8; MS (EI) *m/z* (%) 236 (100), 220, 200, 168, 96.

2-((4-Bromophenyl)thio)phenol (5ae, CAS: 1254831-59-8):[1]



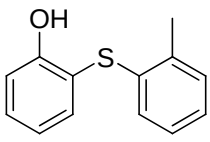
Pale yellow liquid; yield 68%; The product is same as **3ag**.

2-((4-(Trifluoromethyl)phenyl)thio)phenol (5af):



Pale yellow liquid; yield 42%. The product is same as **3ai**.

2-(*o*-Tolylthio)phenol (5ag):[1]



Pale yellow liquid; yield 56%; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.48 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.09-6.95 (m, 4H), 6.66 (d, *J* = 8.0 Hz, 1H), 6.40 (s, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.4, 136.8, 135.7, 134.9, 134.9, 132.0, 130.4, 126.8, 126.2, 126.0, 121.4, 115.6, 20.0; MS (EI) m/z (%) 216 (100), 201, 122, 96, 91.

References

[1] Y. F. Liao, P. C. Jiang, S. P. Chen, H. R. Qi, G. J. Deng, *Green Chem*. **2013**, *15*, 3302.

[2] Z. He, T. F. Jamison, *Angew. Chem., Int. Ed*. **2014**, 53, 3353.

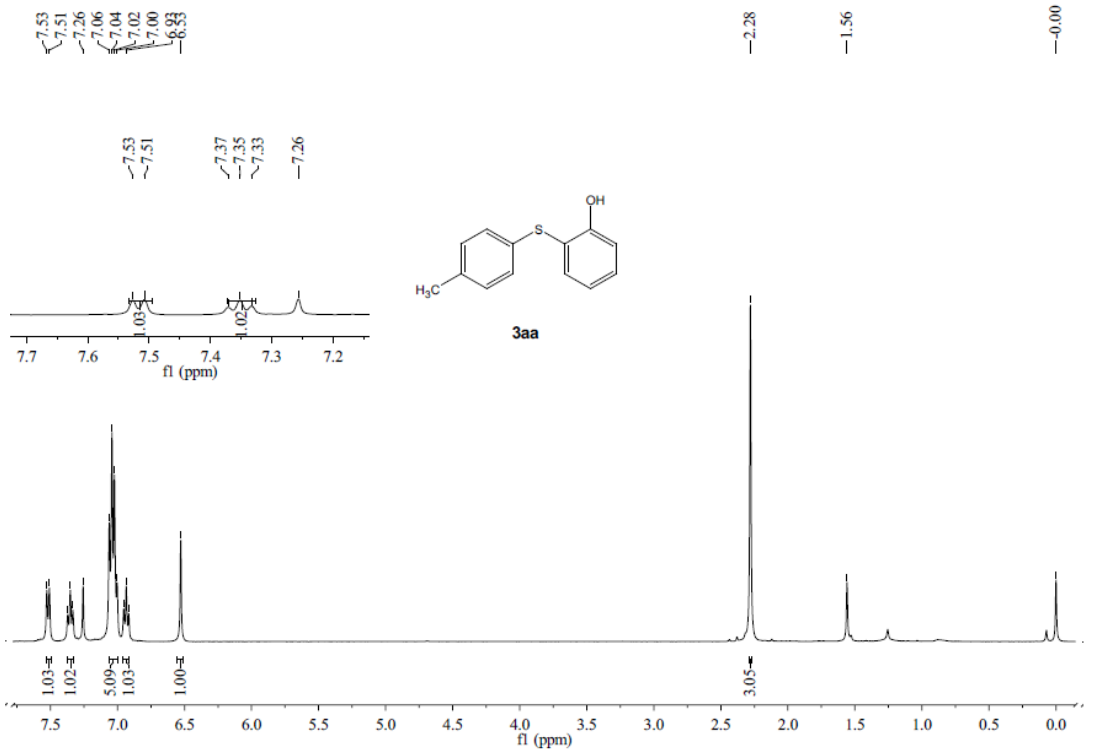
[3] C. Dow, 1965, Patent No US3188352.

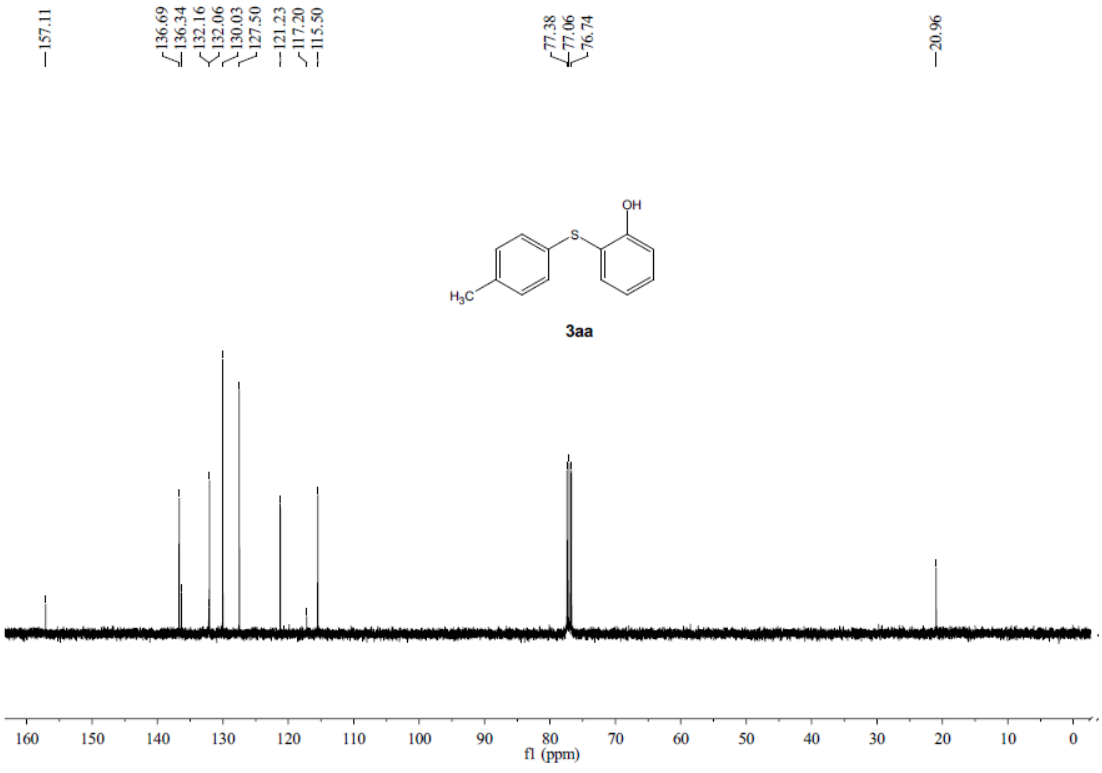
[4] C. Y. Meyers, G Lombardini, L Bonoli, *J. Am. Chem. Soc*. **1962**, 84, 4603.

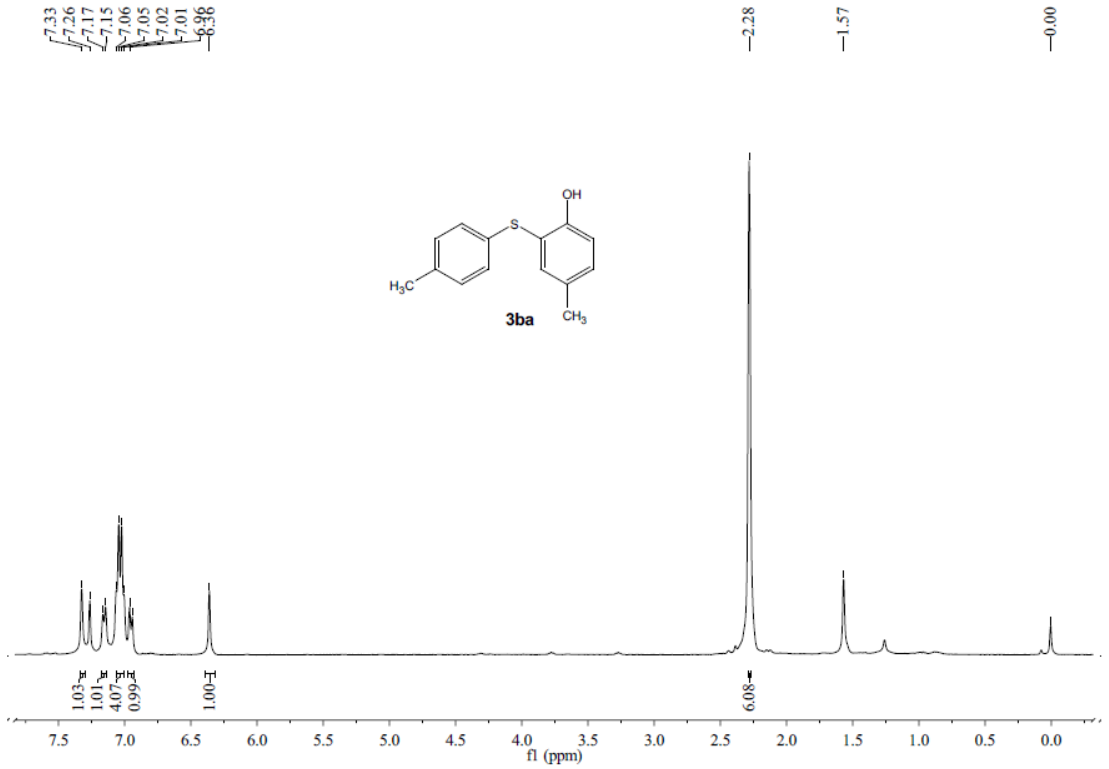
[5] L. Pfizer, P. A. Glossop, D. S. Millan, D. A. Price, 2010, Patent No WO2010/136940A1.

[6] W. E. Parham, G. L. Willette, *J. Org. Chem*. **1960**, 25, 53.

^{1}H NMR and ^{13}C NMR spectra



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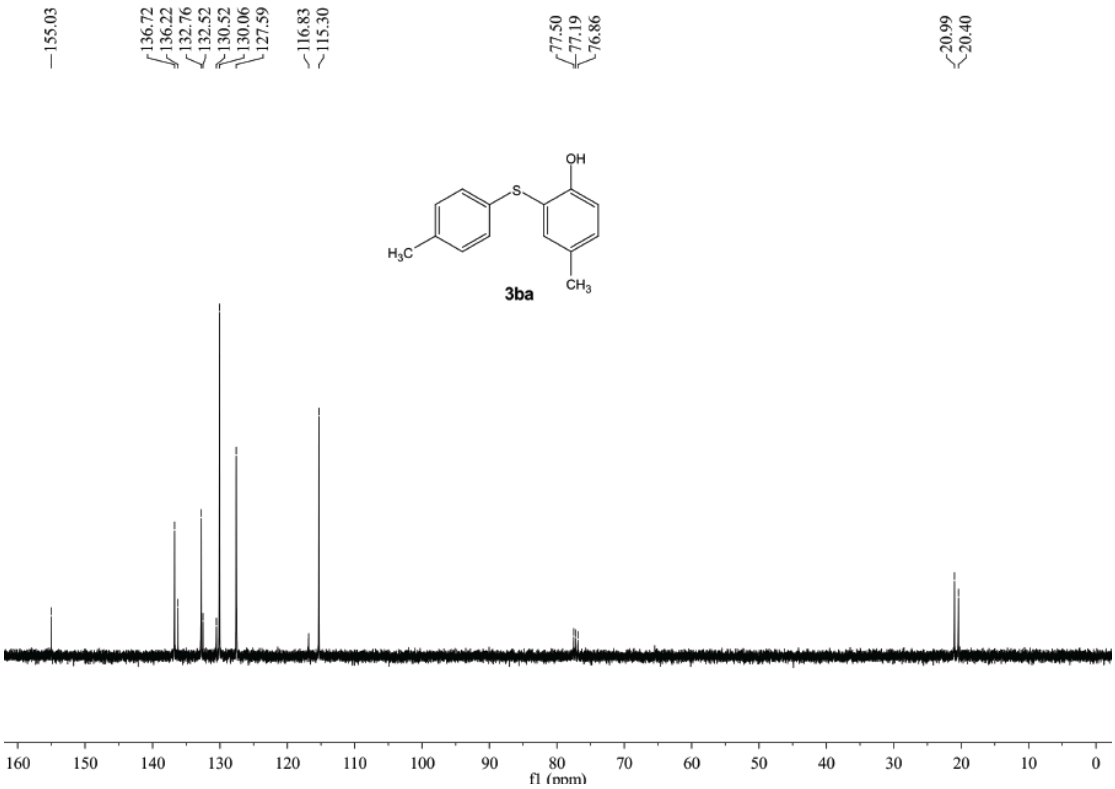
7.26
7.17
7.15
7.06
7.05
7.02
7.01
6.96
6.38
2.28
1.57
0.00
OH
S
H3C
CH3
3ba
1.03
1.01
4.07
0.99
1.00
6.08
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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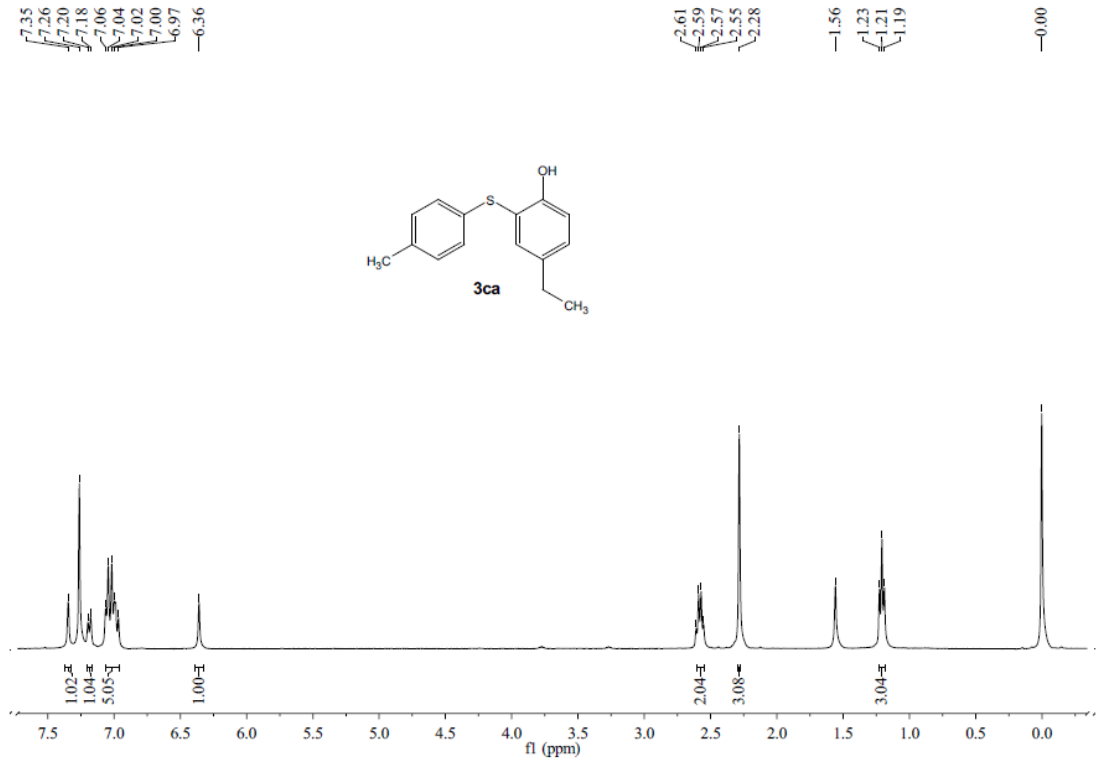
132.52
130.52
130.06
127.59
116.83
115.30
77.50
77.19
76.86
20.99
20.40
OH
S
H3C
CH3
3ba
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.02
7.00
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6.36
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2.57
2.55
2.28
1.56
1.23
1.21
1.19
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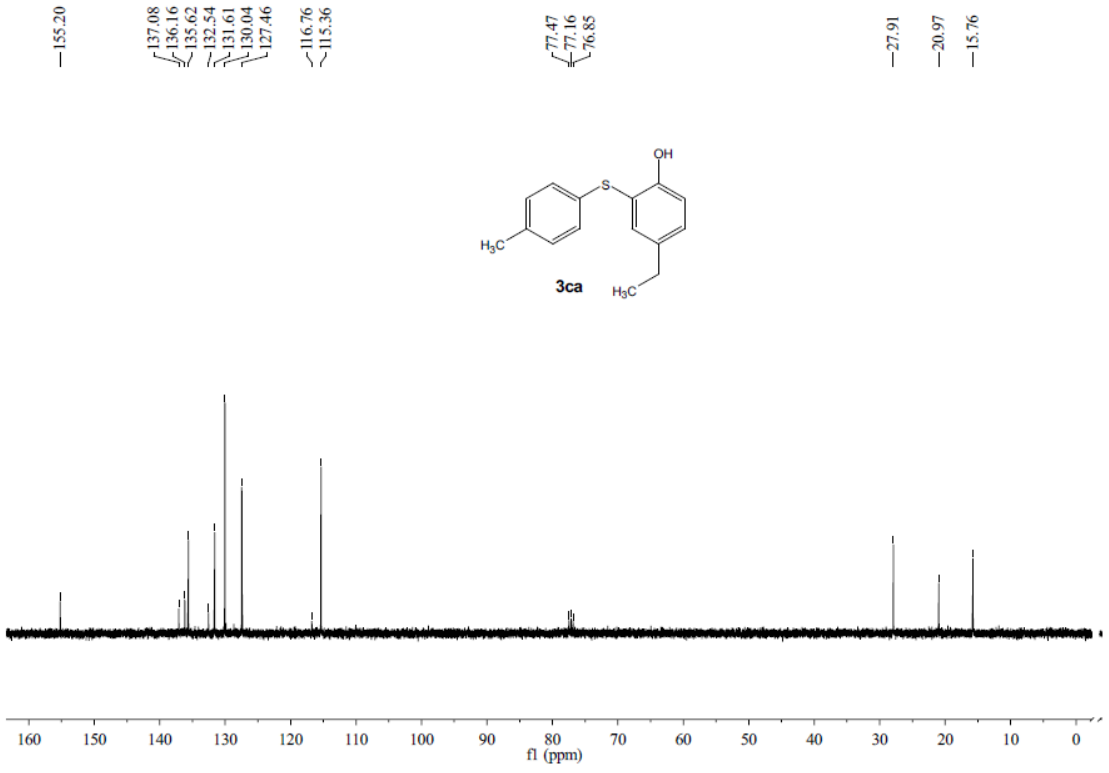
H3C
3ca
CH3
1.02
1.04
5.05
1.00
2.04
3.08
3.04
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.04
127.46
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115.36
77.47
77.16
76.85
27.91
20.97
15.76
OH
S
H3C
3ca
H3C
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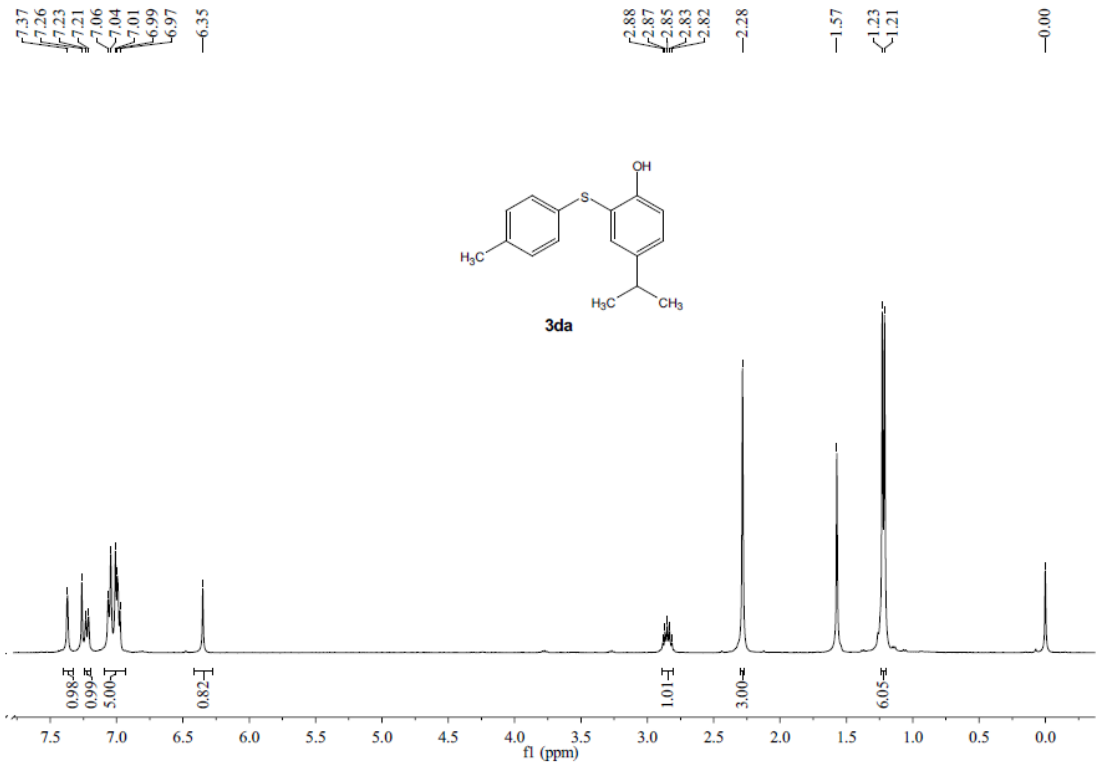
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.0
6.5
6.0
5.5
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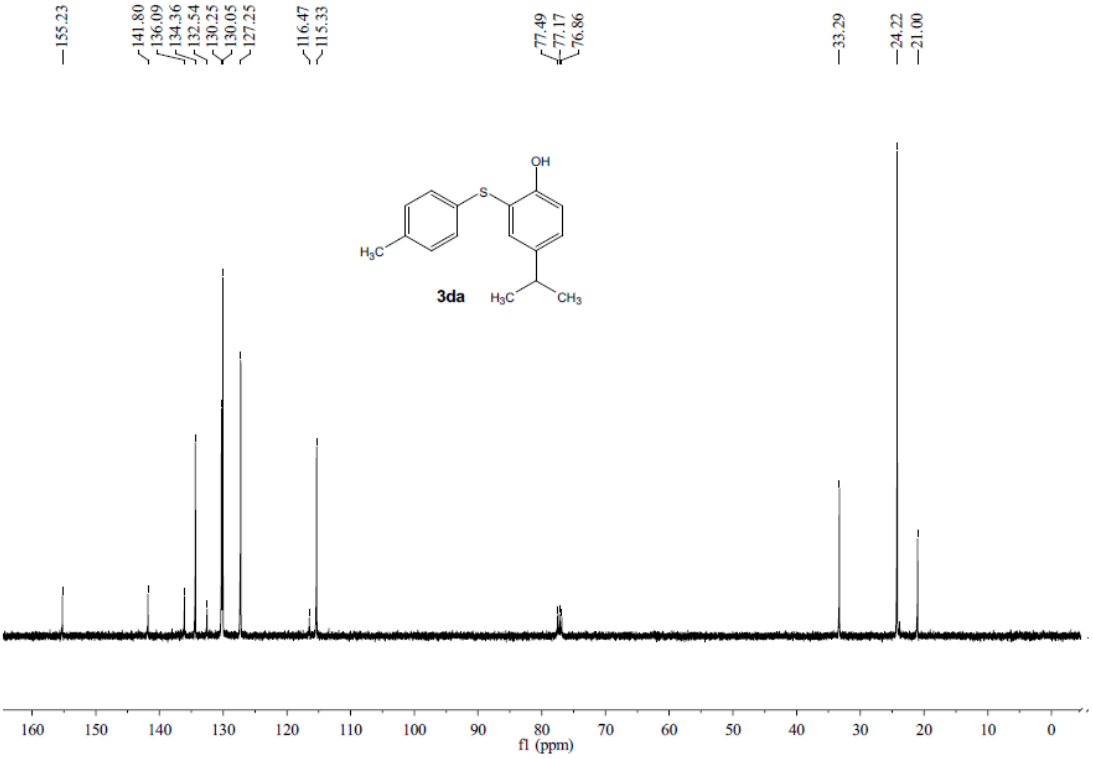
0.0
f1 (ppm)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33.29
24.22
21.00
OH
S
H3C
3da
H3C
CH3
160
150
140
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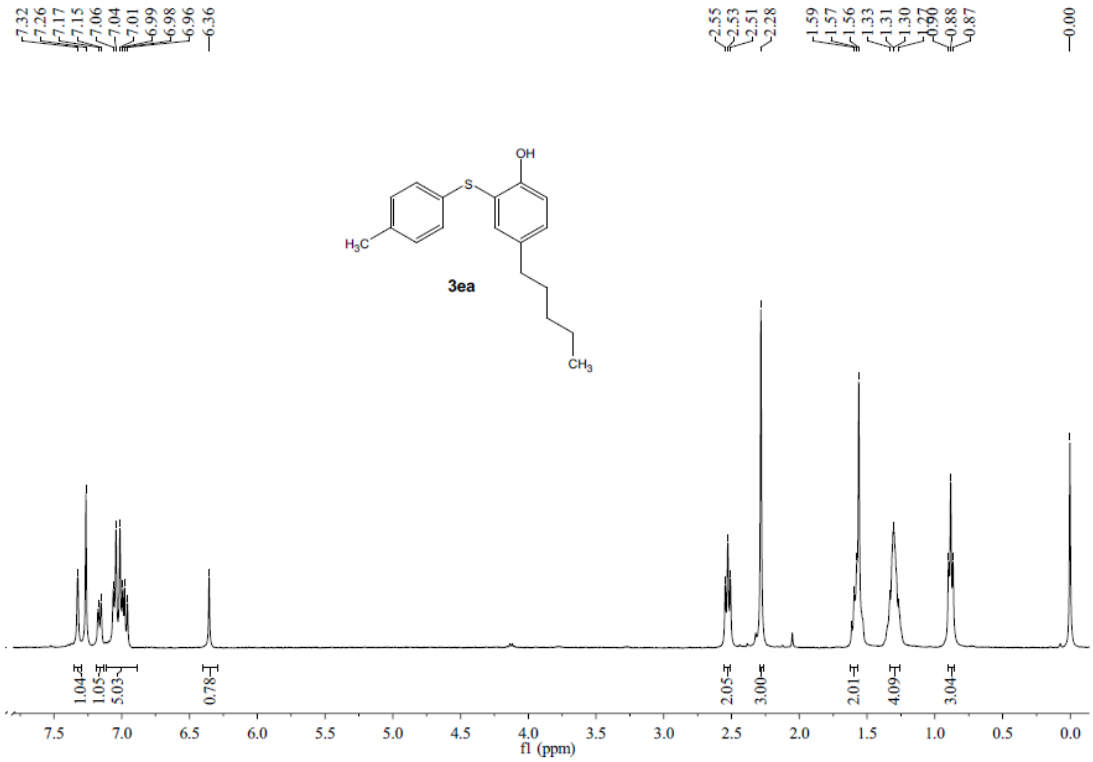
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7.04
7.01
6.99
6.98
6.96
6.36
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2.53
2.51
2.28
1.59
1.57
1.56
1.33
1.31
1.30
1.27
0.90
0.88
0.87
0.00
OH
S
H3C
3ea
CH3
1.04
1.05
5.03
0.78
2.05
3.00
2.01
4.09
3.04
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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1.0
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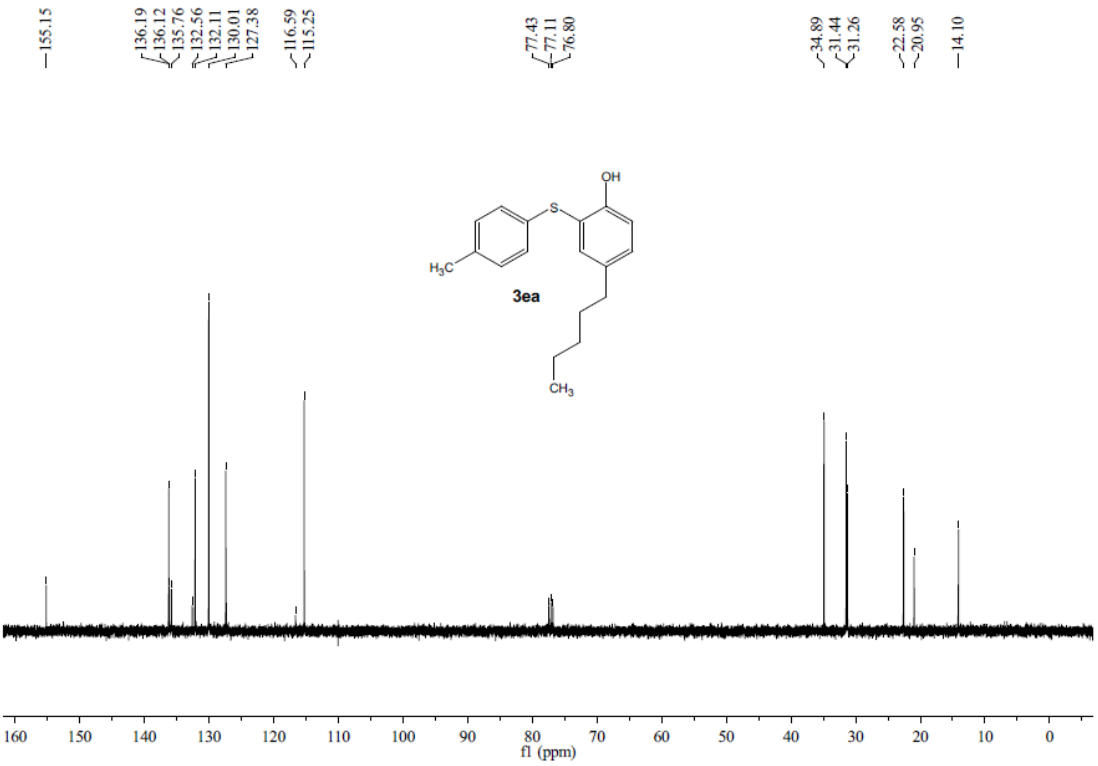
0.0
f1 (ppm)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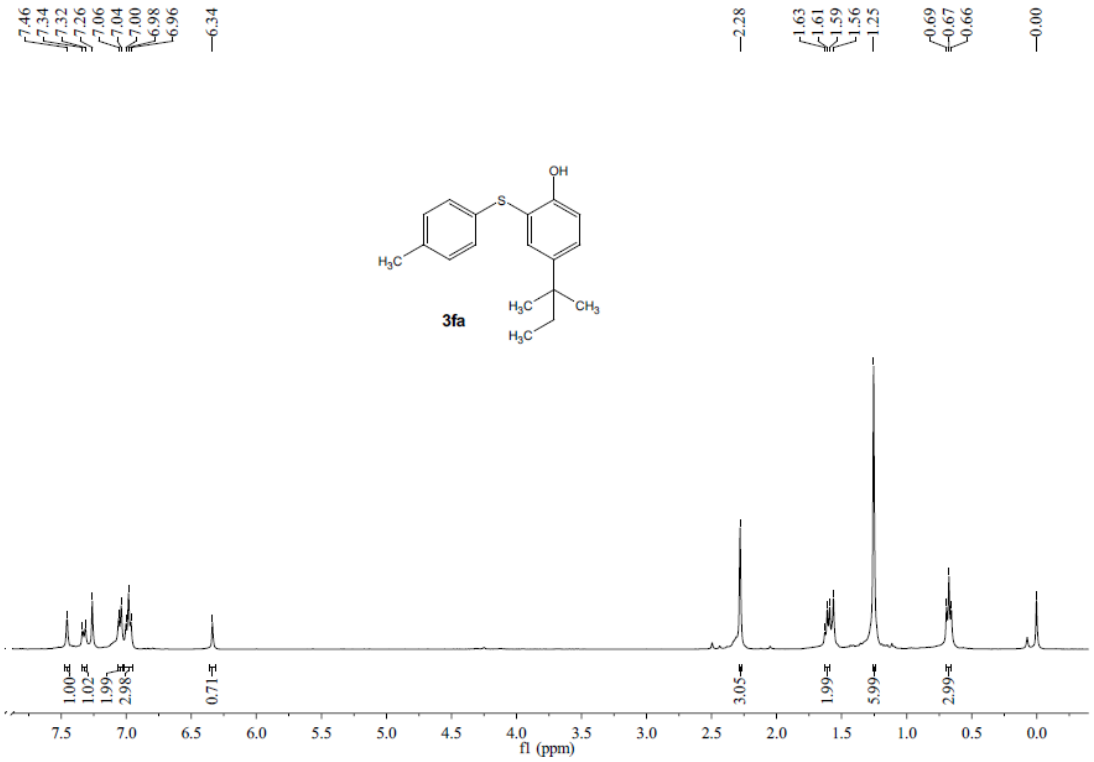
132.11
130.01
127.38
116.59
115.25
77.43
77.11
76.80
34.89
31.44
31.26
22.58
20.95
14.10
OH
S
H3C
3ea
CH3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.34
2.28
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1.61
1.59
1.56
1.25
0.69
0.67
0.66
0.00
OH
S
H3C
H3C
CH3
H3C
3fa
1.00
1.02
1.99
2.98
0.71
3.05
1.99
5.99
2.99
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
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2.5
2.0
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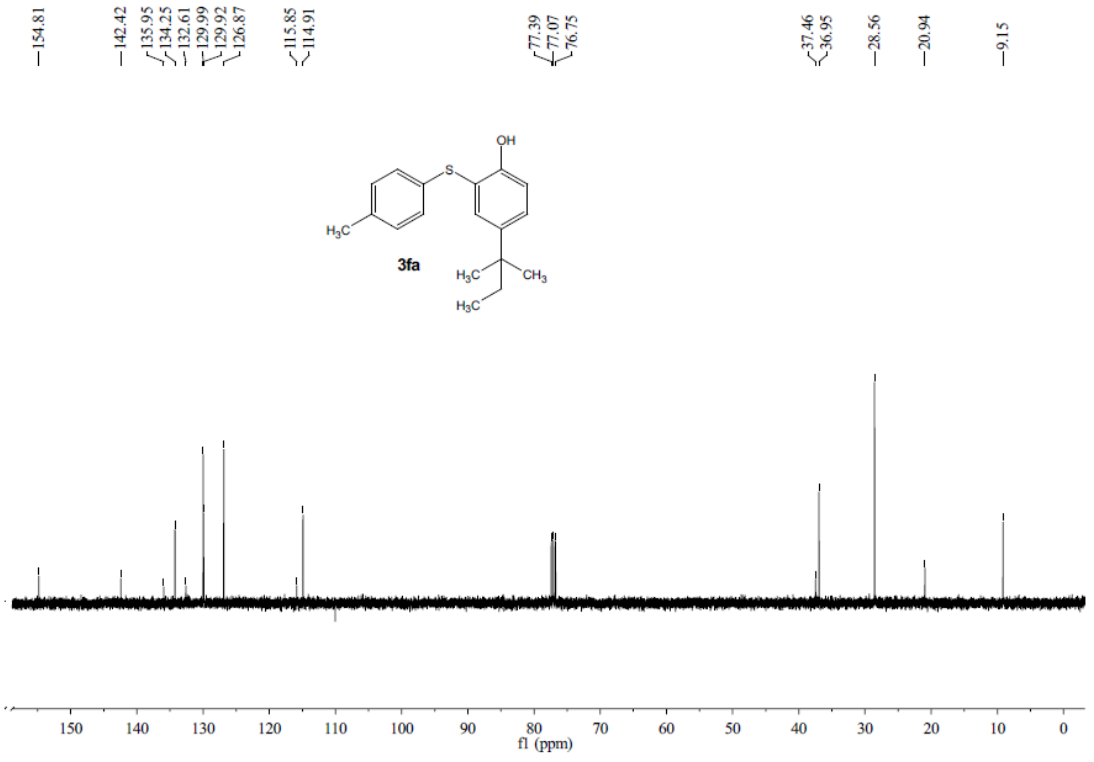
0.0
f1 (ppm)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77.39
77.07
76.75
37.46
36.95
28.56
20.94
9.15
OH
S
H3C
H3C
CH3
H3C
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130
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100
90
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50
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30
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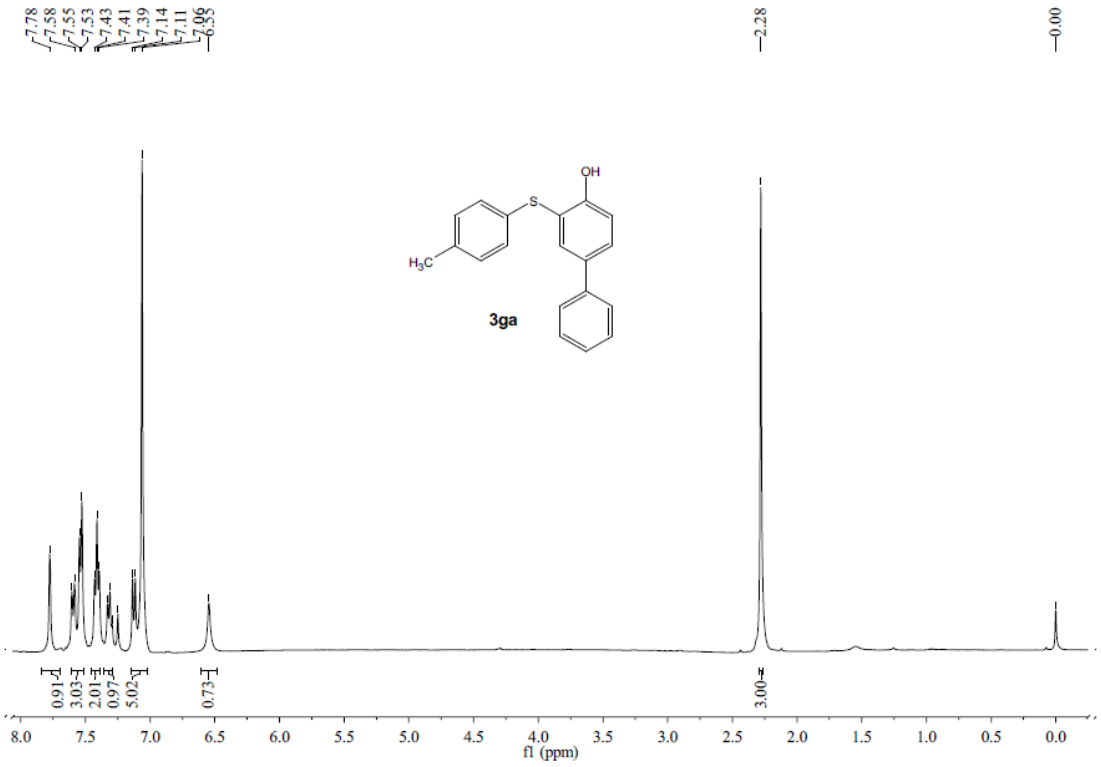
10
0
f1 (ppm)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7.41
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7.14
7.11
7.06
6.95
2.28
0.00
OH
S
H3C
3ga
0.91
3.03
2.01
0.97
5.02
0.73
3.00
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
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1.0
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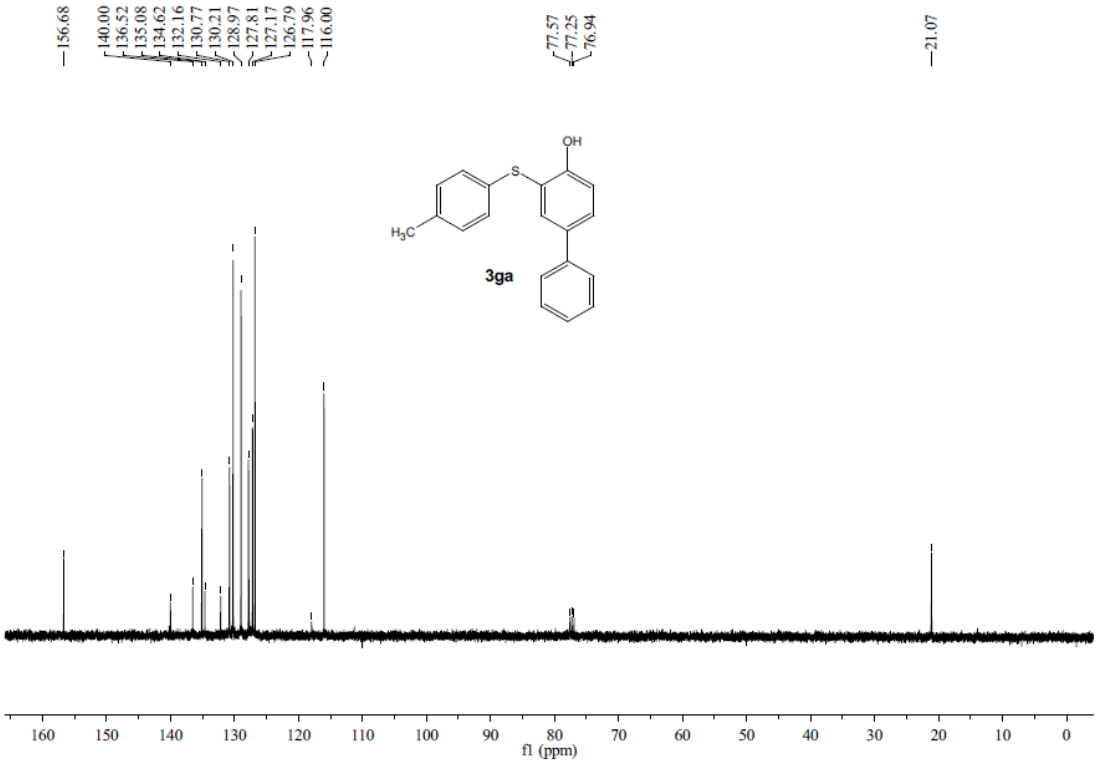
0.0
f1 (ppm)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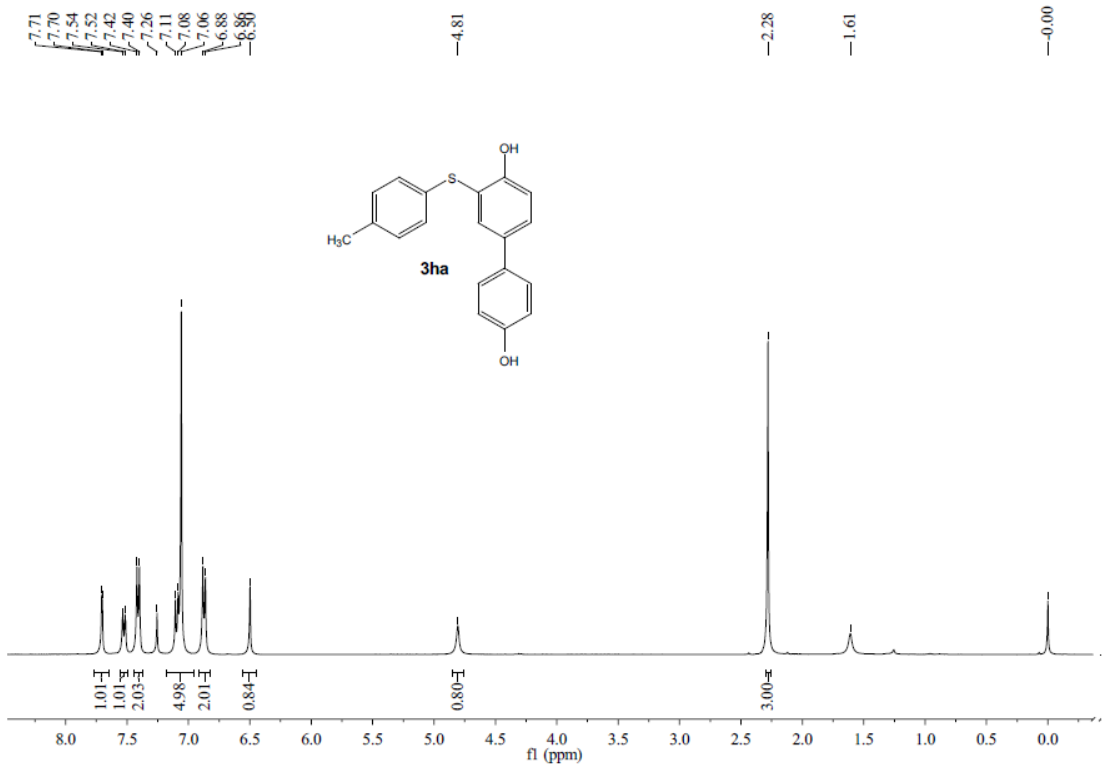
130.21
128.97
127.81
127.17
126.79
117.96
116.00
77.57
77.25
76.94
21.07
OH
S
H3C
3ga
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.52
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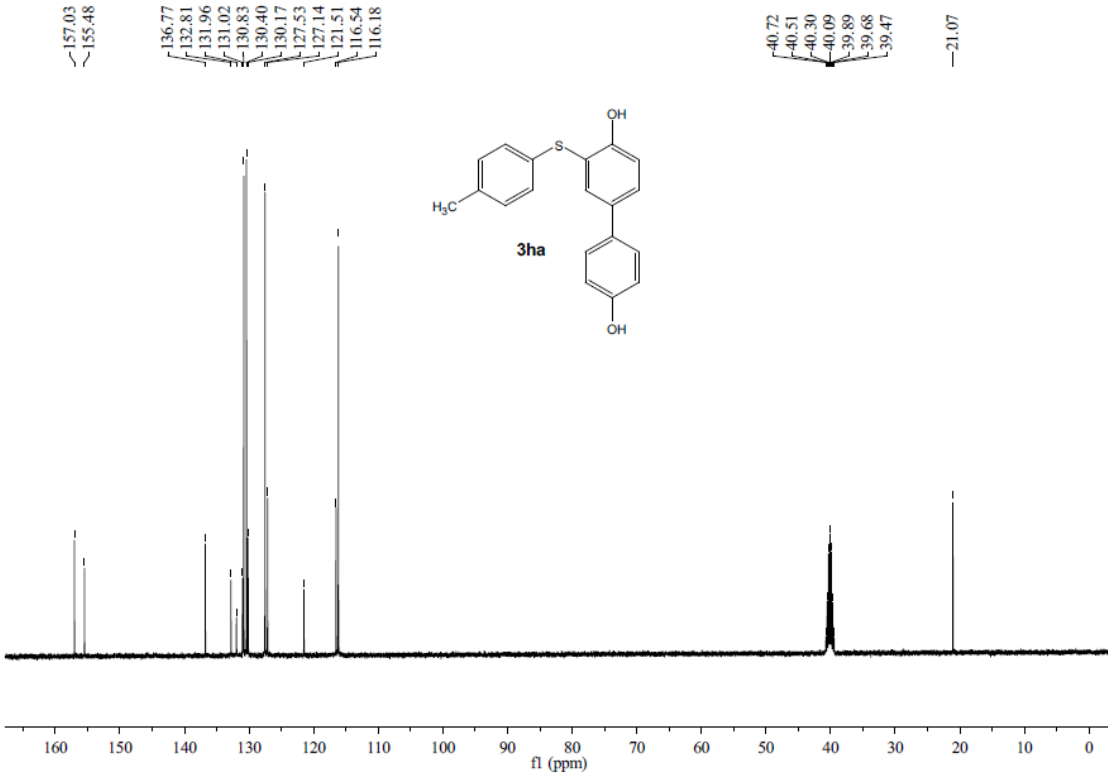
7.40
7.26
7.11
7.08
7.06
6.88
6.86
6.30
4.81
2.28
1.61
0.00
OH
S
H3C
3ha
OH
1.01
1.01
2.03
4.98
2.01
0.84
0.80
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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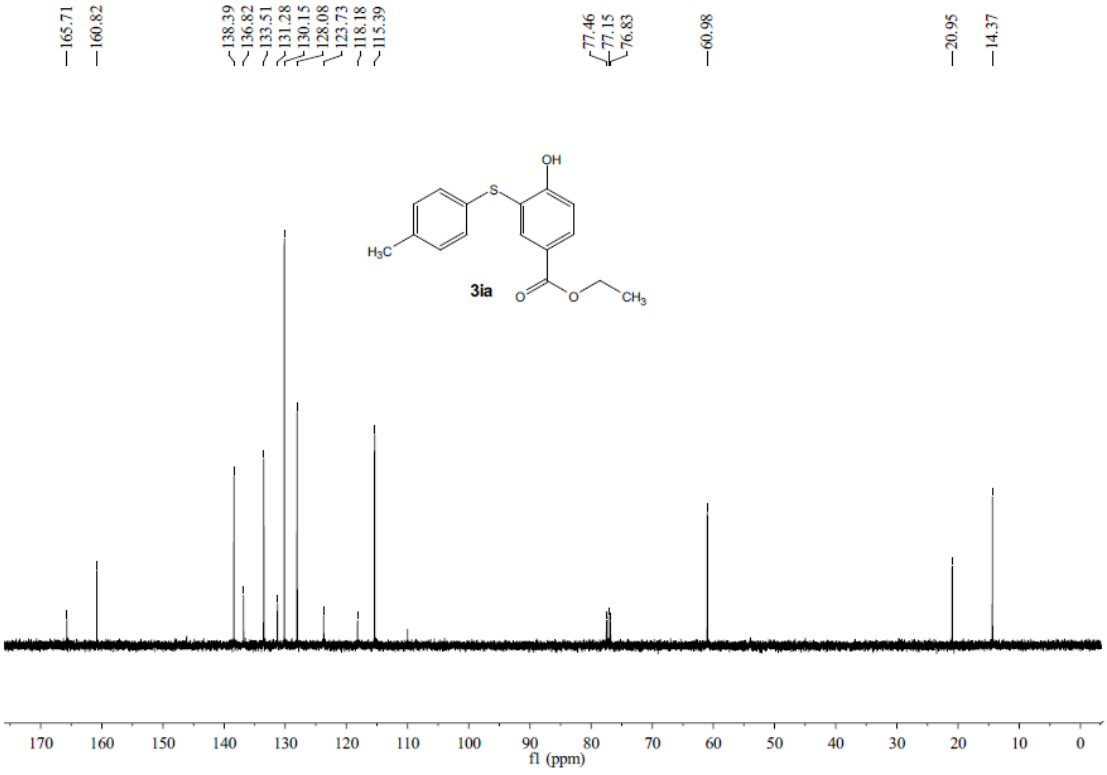
131.96
131.02
130.83
130.40
130.17
127.53
127.14
121.51
116.54
116.18
40.72
40.51
40.30
40.09
39.89
39.68
39.47
21.07
OH
S
H3C
3ha
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.27
8.06
8.04
7.26
7.09
7.06
7.04
7.03
6.95
4.37
4.35
4.34
4.32
2.29
1.58
1.39
1.38
1.36
0.00
OH
S
H3C
O
O
CH3
3ia
1.00
1.03
5.07
0.98
2.05
3.03
3.00
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
0.0
f1 (ppm)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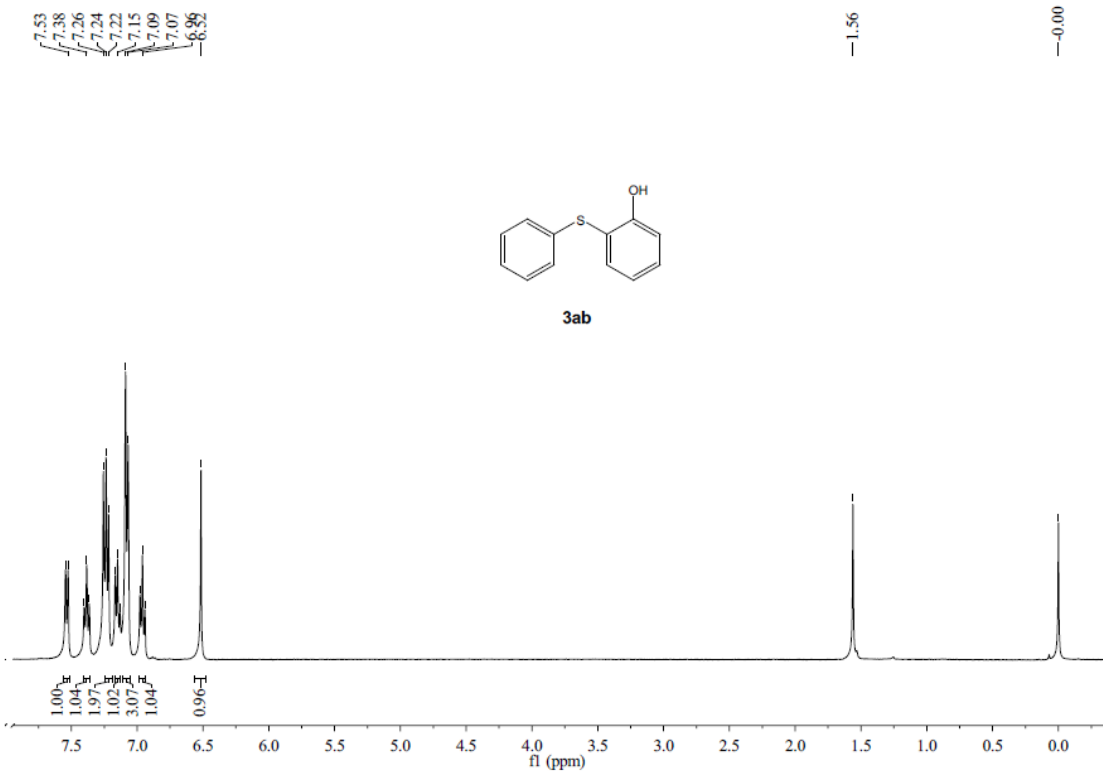
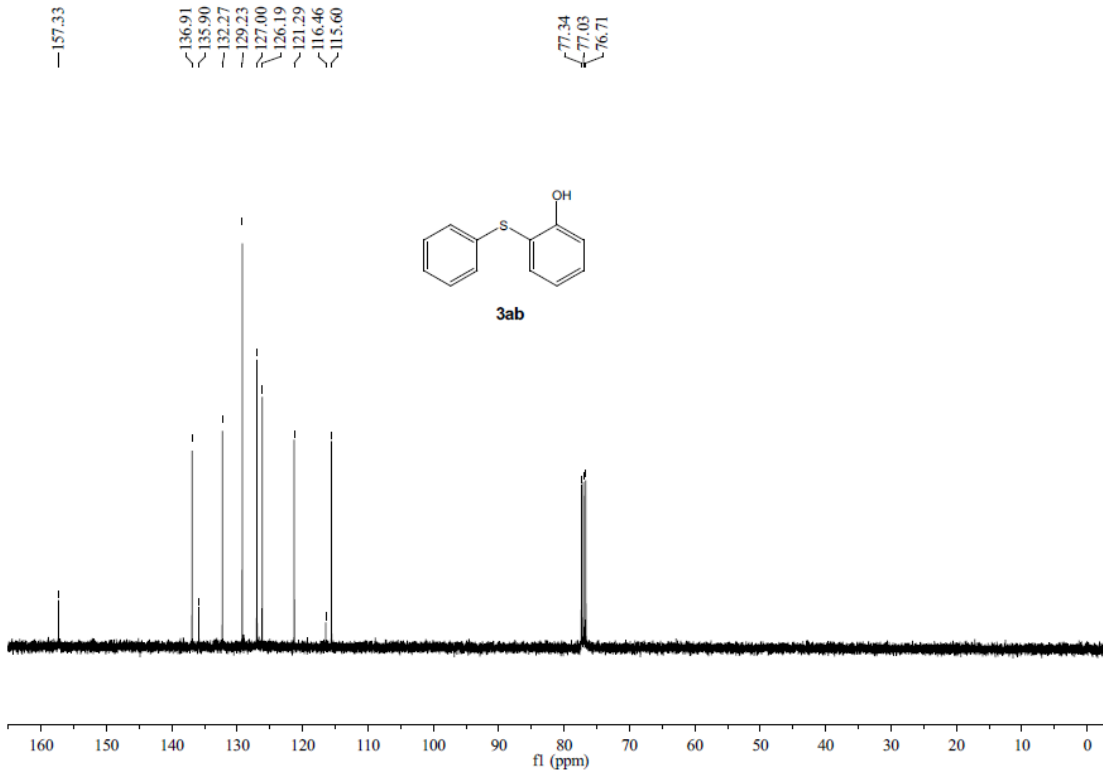
131.28
130.15
128.08
123.73
118.18
115.39
77.46
77.15
76.83
60.98
20.95
14.37
OH
S
H3C
O
O
CH3
3ia
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.53
7.38
7.26
7.24
7.22
7.15
7.09
7.07
6.96
6.92
1.56
0.00
OH
S
3ab
1.00
1.04
1.97
1.02
3.07
1.04
0.96
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
0.0
f1 (ppm)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136.91
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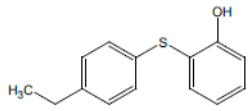
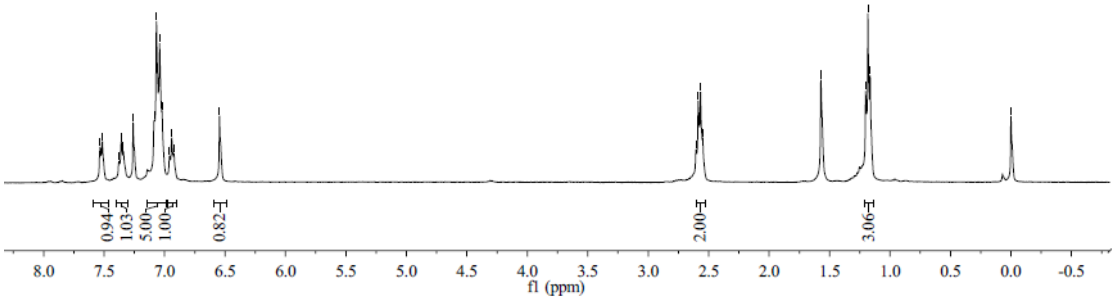
129.23
127.00
126.19
121.29
116.46
115.60
77.34
77.03
76.71
OH
S
3ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.53
7.51
7.36
7.34
7.26
7.08
7.07
7.04
7.02
6.94
6.92
6.55
2.61
2.59
2.57
2.55
1.57
1.20
1.18
1.16
0.00


OH
S
H3C

3ac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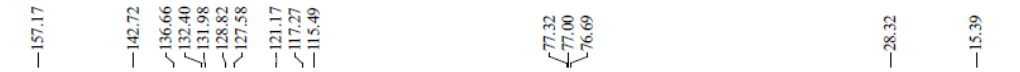
1.03
5.00
1.00
0.82
2.00
3.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.58
121.17
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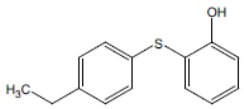
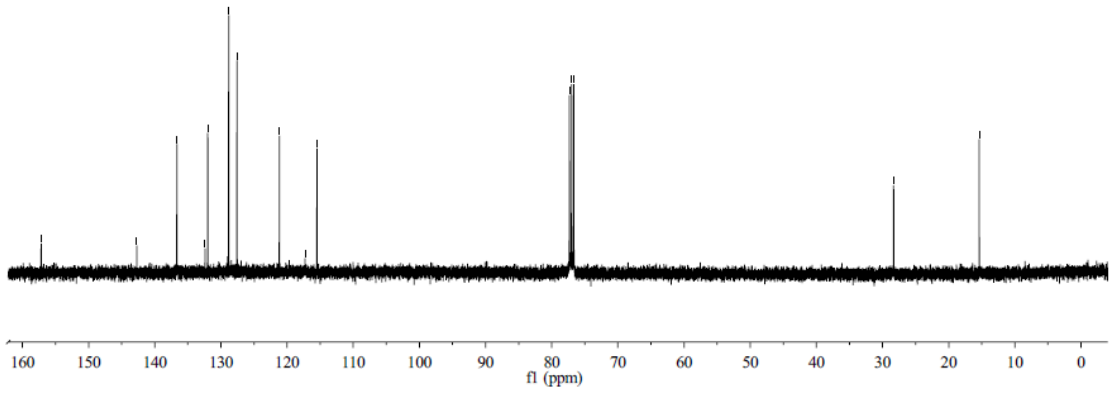
77.32
77.00
76.69
28.32
15.39


OH
S
H3C

3ac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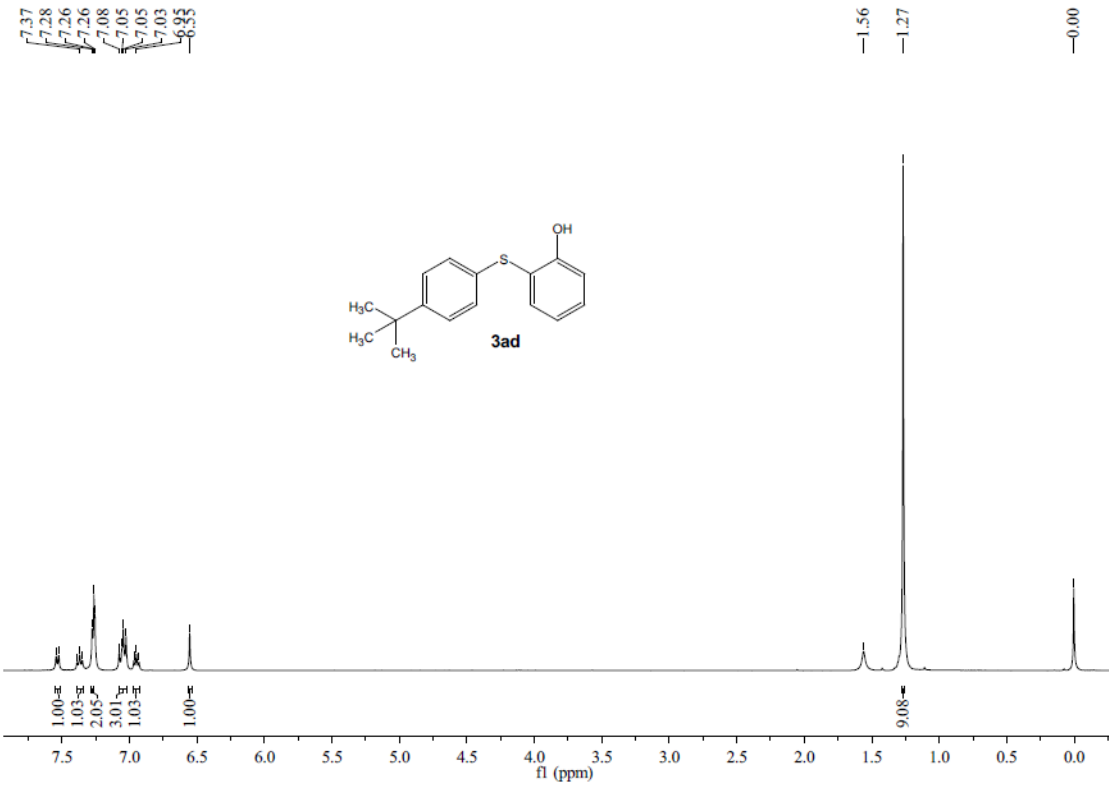
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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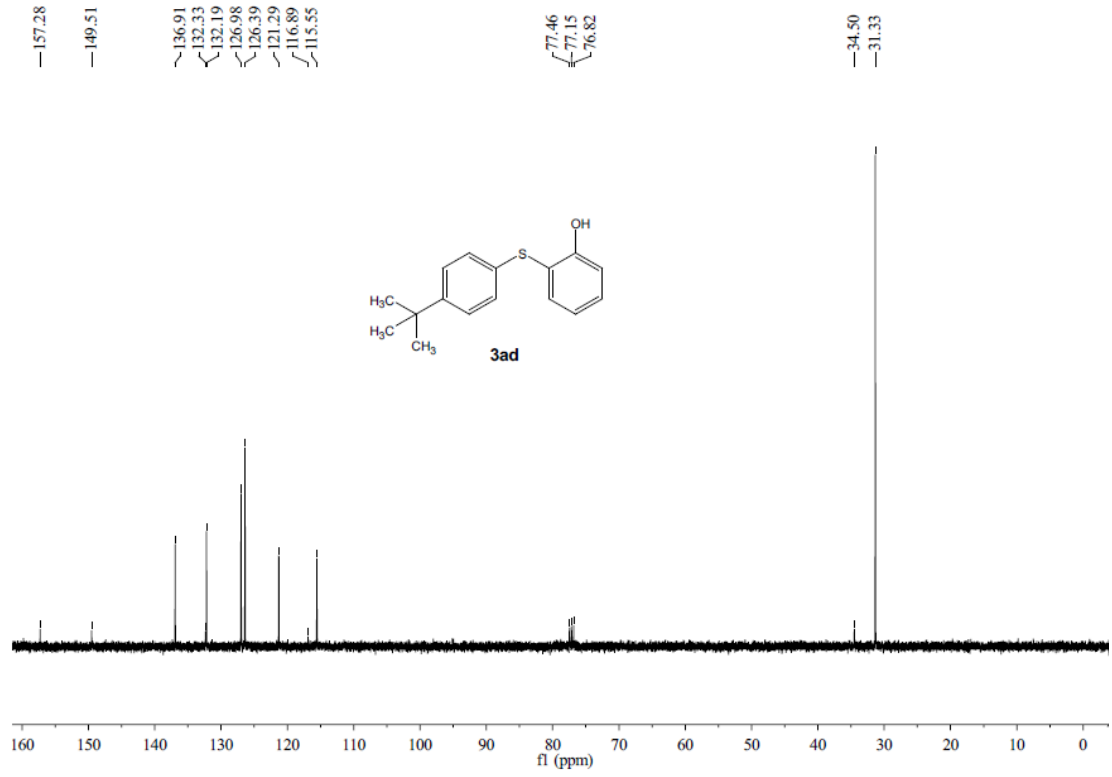
7.28
7.26
7.26
7.08
7.05
7.05
7.03
6.95
6.55
1.56
1.27
0.00
OH
S
H3C
H3C
CH3
3ad
1.00
1.03
2.05
3.01
1.03
1.00
9.08
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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121.29
116.89
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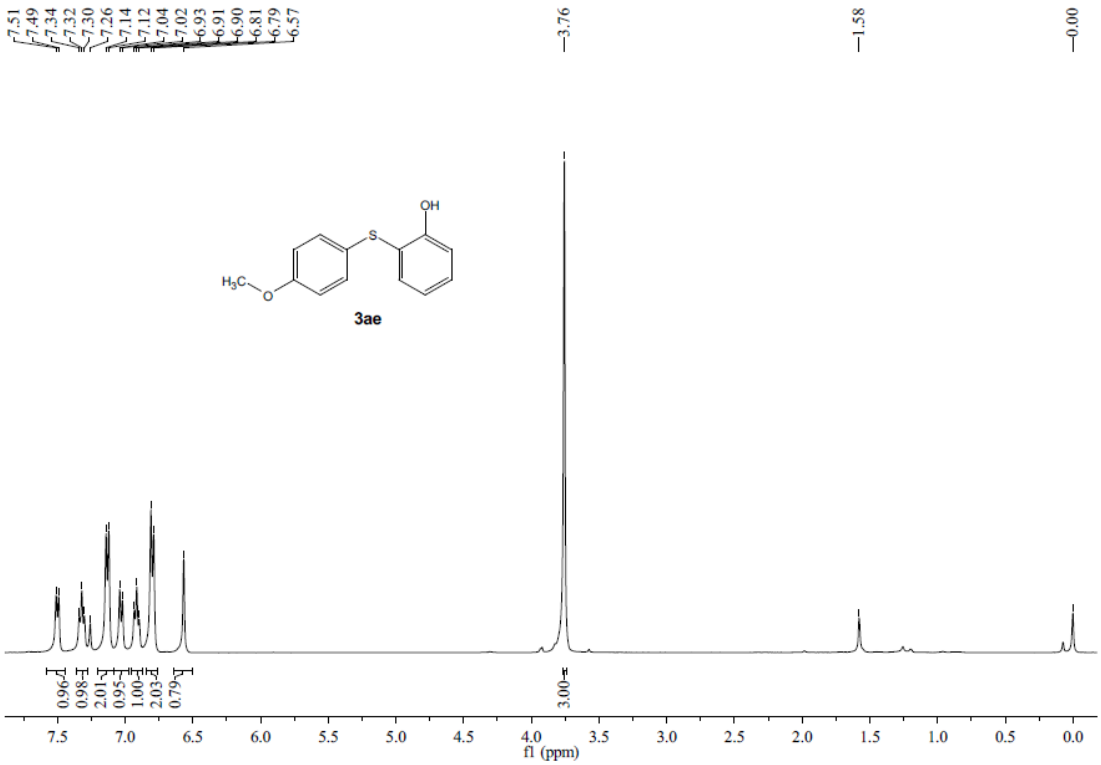
77.46
77.15
76.82
34.50
31.33
OH
S
H3C
H3C
CH3
3ad
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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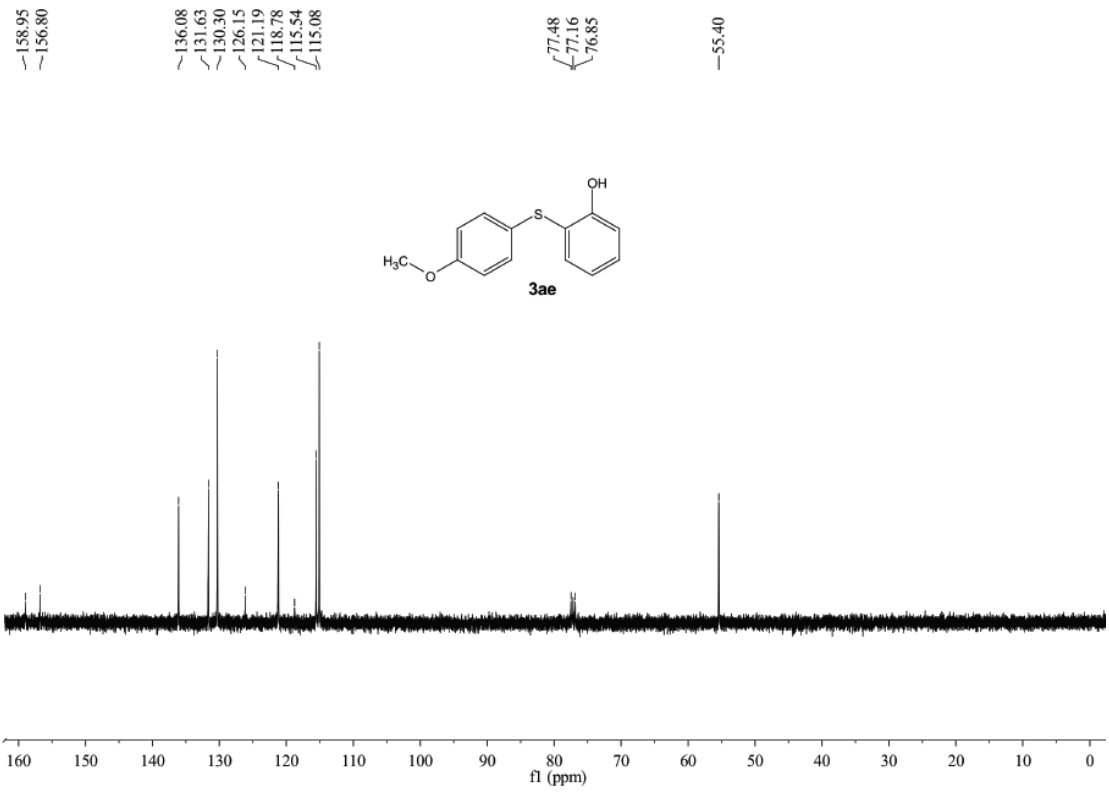
7.49
7.34
7.32
7.30
7.26
7.14
7.12
7.04
7.02
6.93
6.91
6.90
6.81
6.79
6.57
3.76
1.58
0.00
OH
S
H3C
O
3ae
0.96
0.98
2.01
0.95
1.00
2.03
0.79
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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118.78
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115.08
77.48
77.16
76.85
55.40
OH
S
H3C
O
3ae
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150
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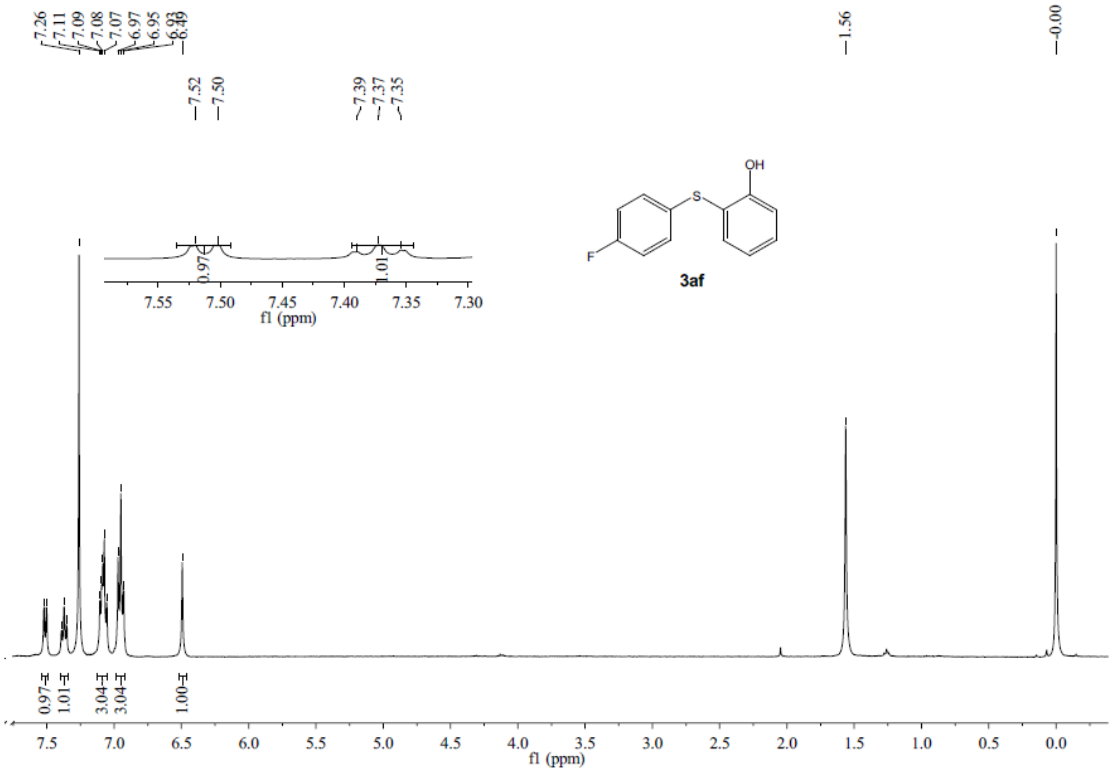
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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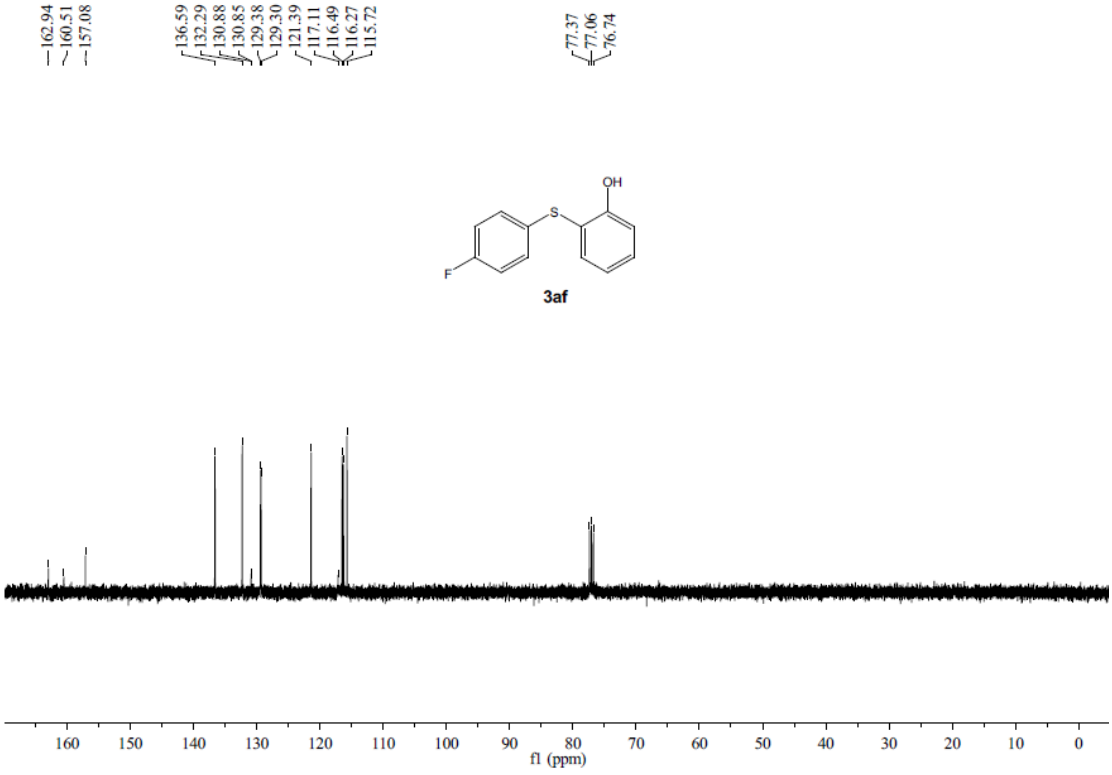
7.08
7.07
6.97
6.95
6.93
6.49
7.52
7.50
7.39
7.37
7.35
1.56
0.00
OH
S
F
3af
0.97
1.01
7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)
0.97
1.01
3.04
3.04
1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.39
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116.49
116.27
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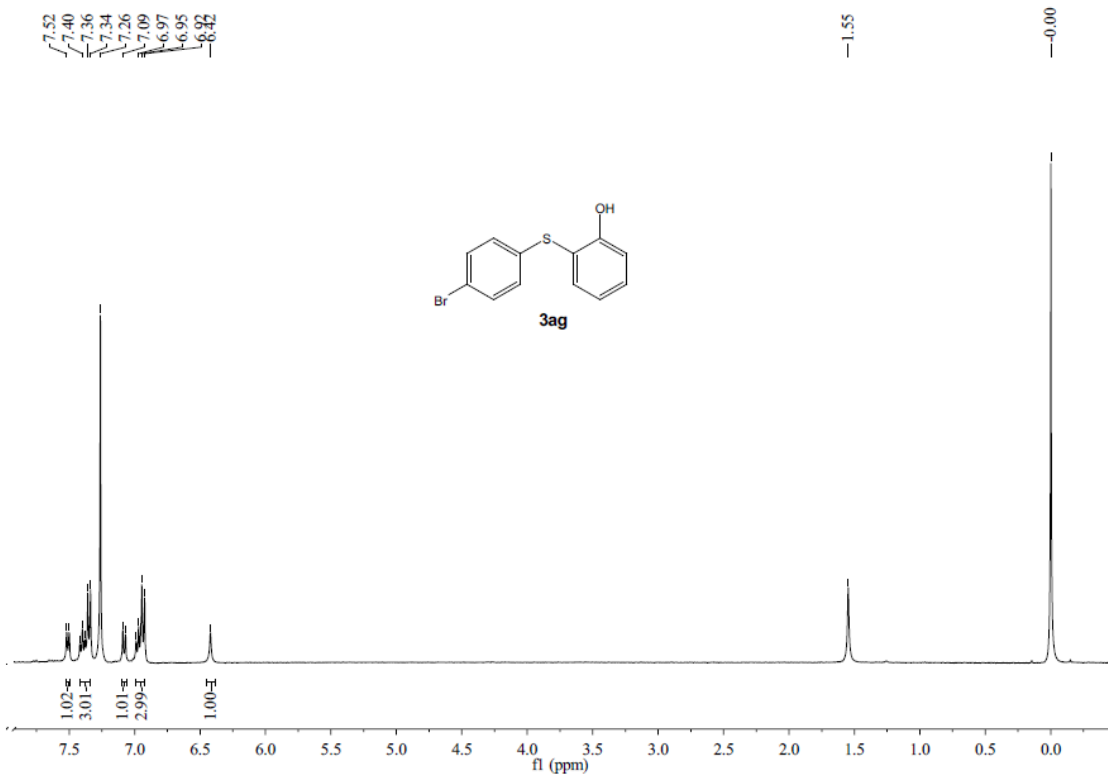
77.37
77.06
76.74
OH
S
F
3af
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.36
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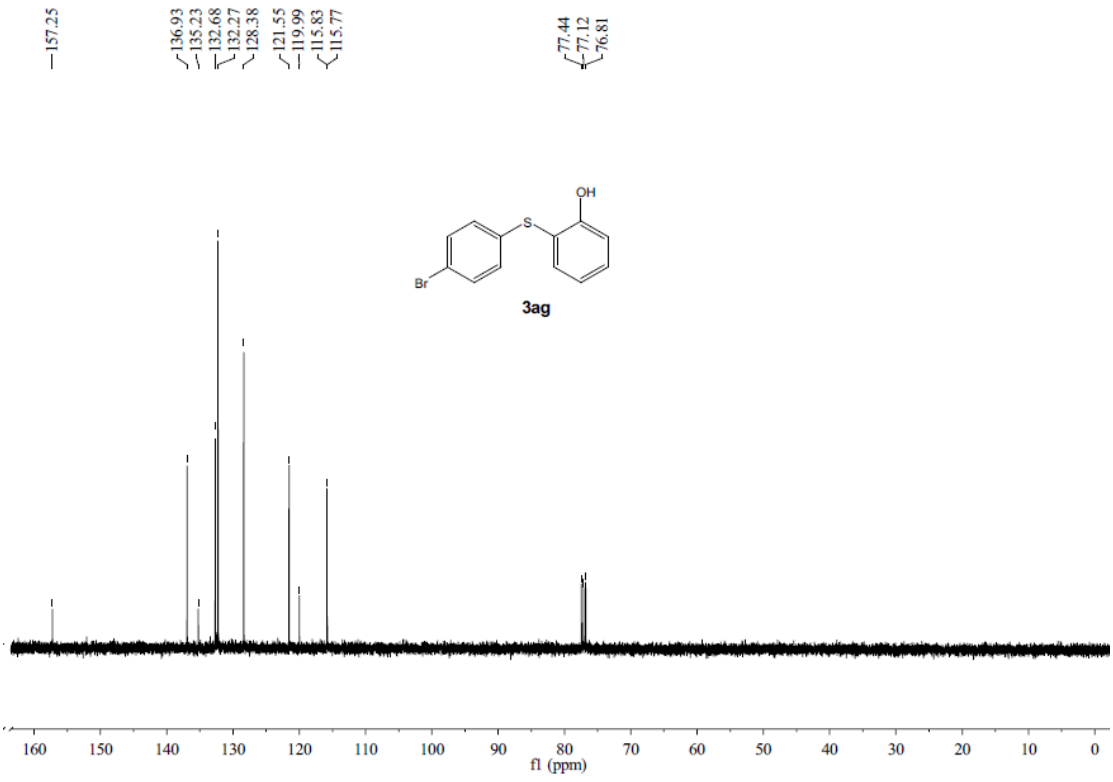
7.26
7.09
6.97
6.95
6.92
6.42
1.55
0.00
OH
S
Br
3ag
1.02
3.01
1.01
2.99
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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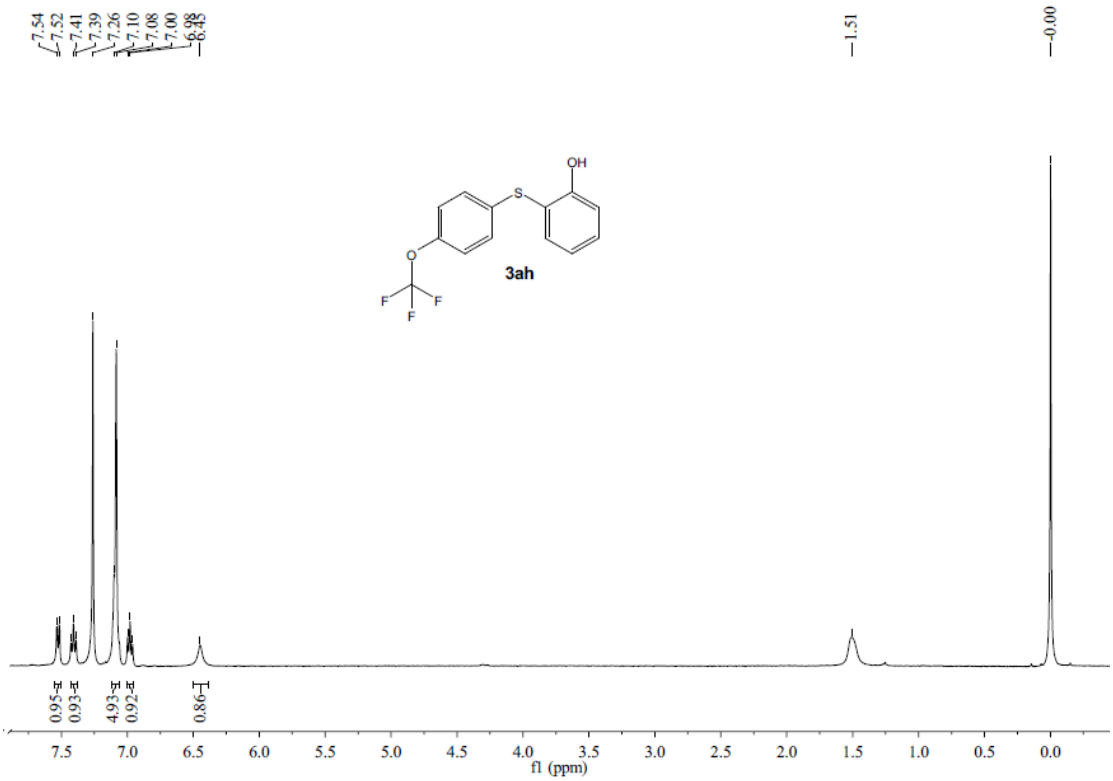
128.38
121.55
119.99
115.83
115.77
77.44
77.12
76.81
OH
S
Br
3ag
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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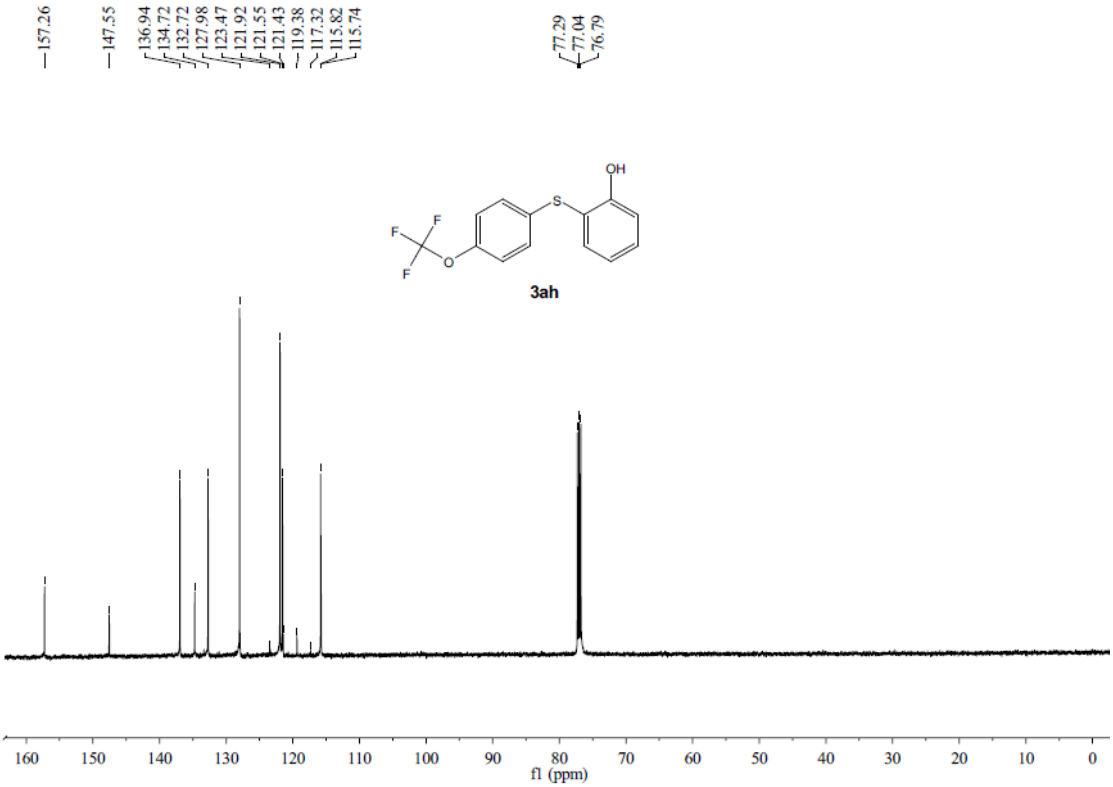
7.10
7.08
7.00
6.98
6.45
1.51
0.00
OH
S
O
F
F
F
3ah
0.95
0.93
4.93
0.92
0.86
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.98
123.47
121.92
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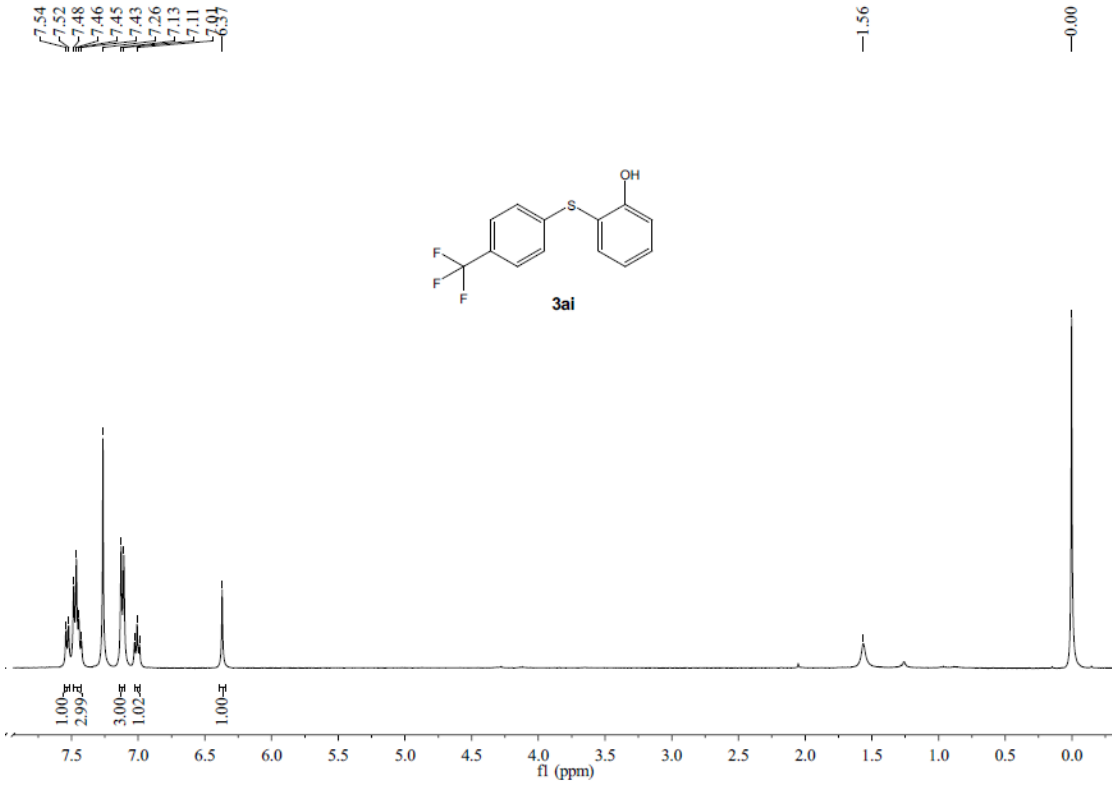
121.43
119.38
117.32
115.82
115.74
77.29
77.04
76.79
OH
S
O
F
F
F
3ah
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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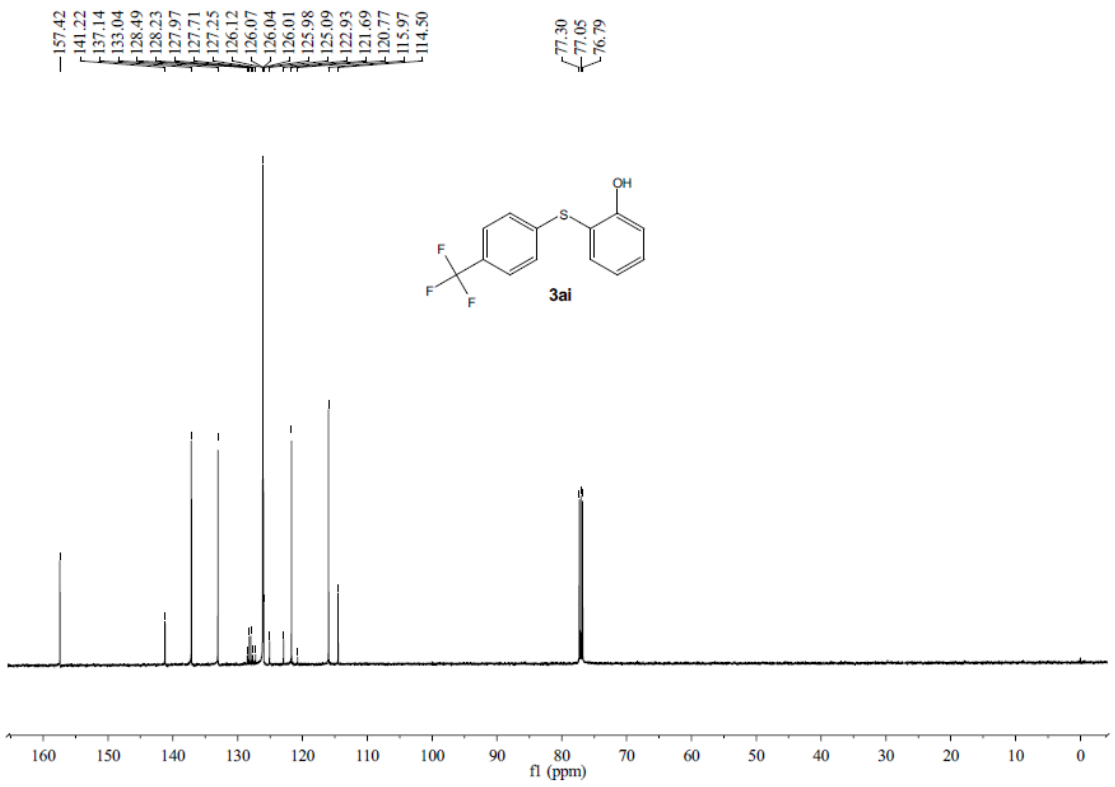
7.52
7.48
7.46
7.45
7.43
7.26
7.13
7.11
7.01
6.97
1.56
0.00
OH
S
F
F
F
3ai
1.00
2.99
3.00
1.02
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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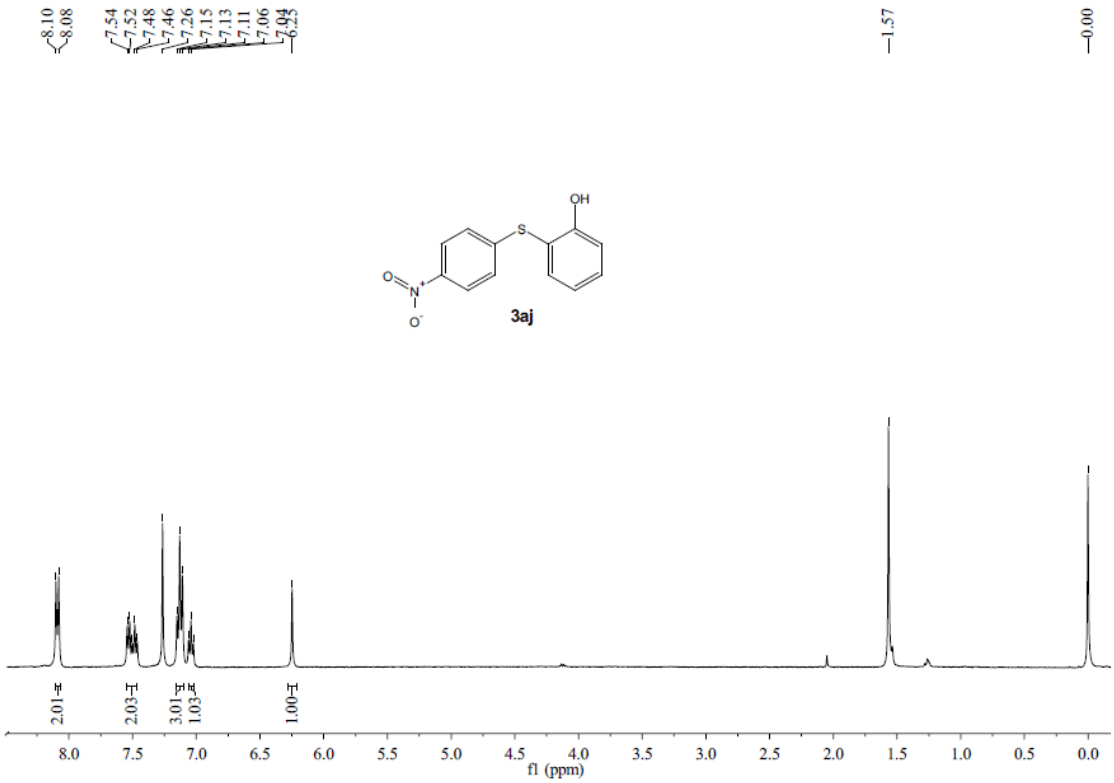
141.22
137.14
133.04
128.49
128.23
127.97
127.71
127.25
126.12
126.07
126.04
126.01
125.98
125.09
122.93
121.69
120.77
115.97
114.50
77.30
77.05
76.79
OH
S
F
F
F
3ai
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.08
7.54
7.52
7.48
7.46
7.26
7.15
7.13
7.11
7.06
7.04
6.23
1.57
0.00
OH
S
O
N
O
3aj
2.01
2.03
3.01
1.03
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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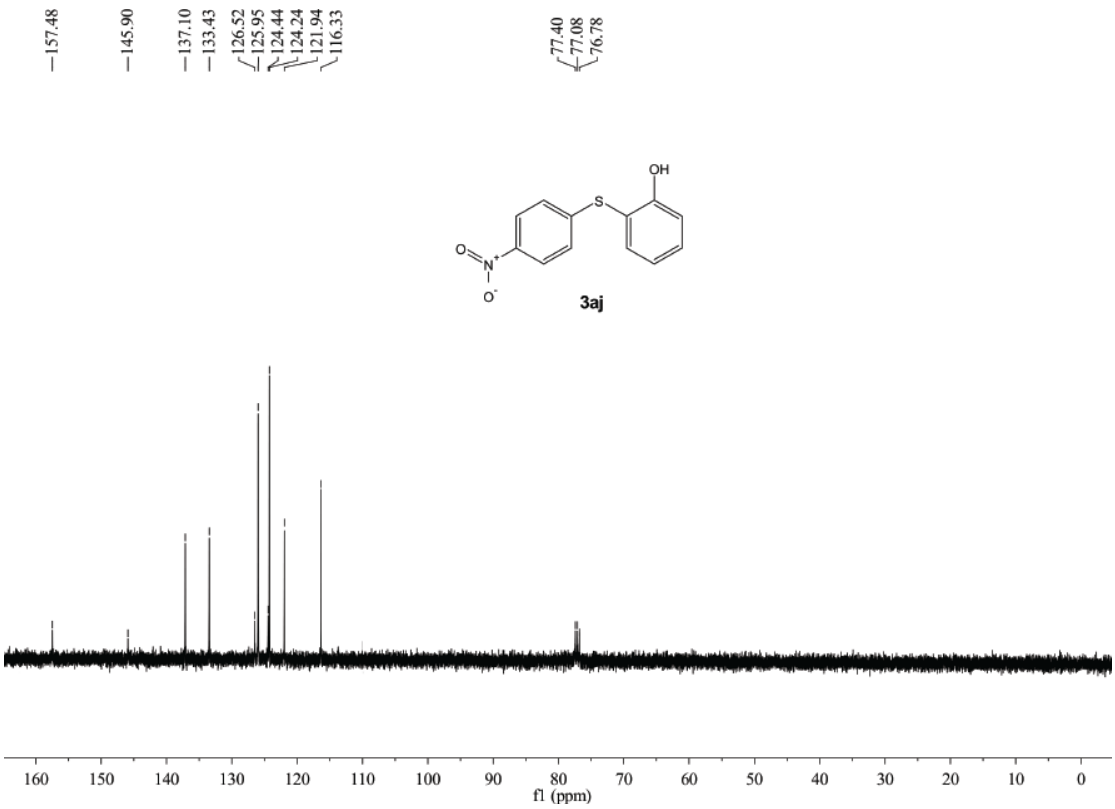
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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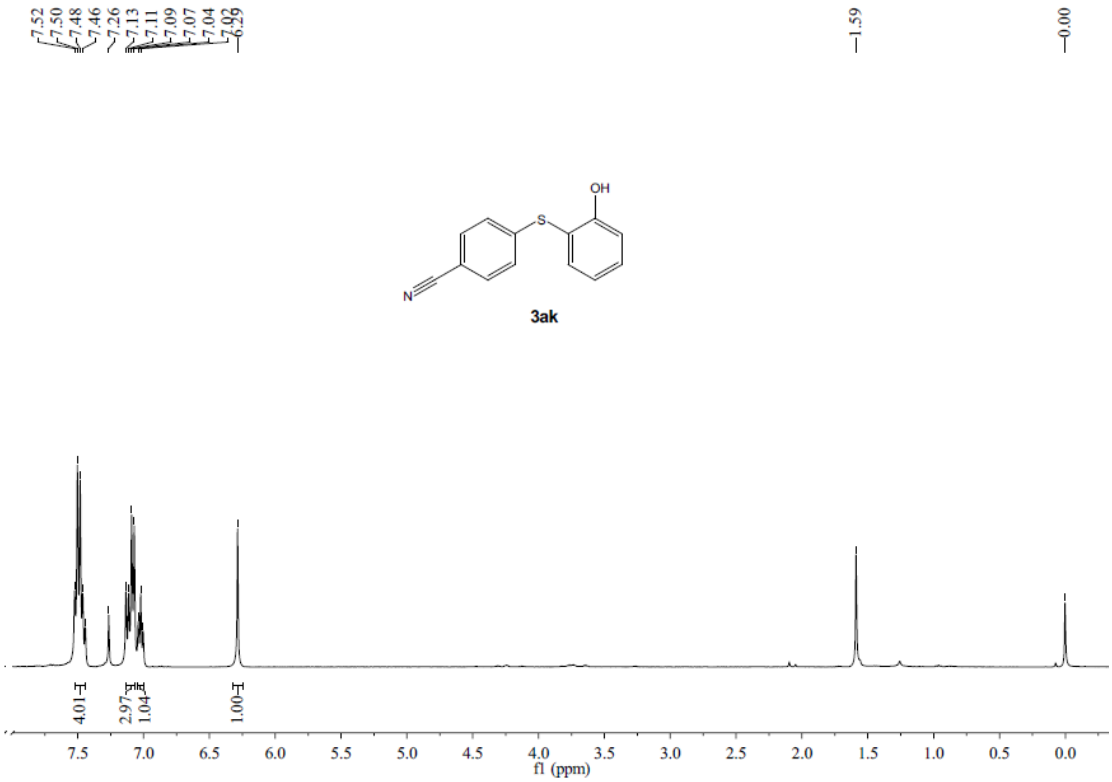
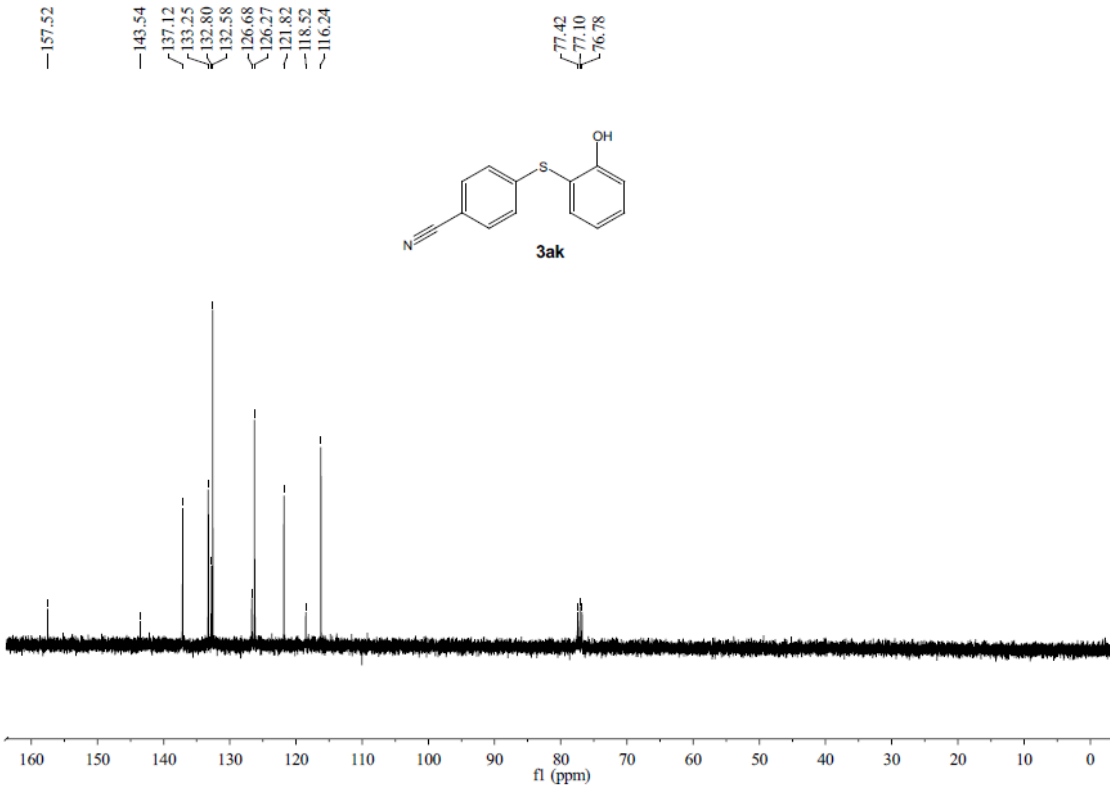
126.52
125.95
124.44
124.24
121.94
116.33
77.40
77.08
76.78
OH
S
O
N
O
3aj
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.52
7.50
7.48
7.46
7.26
7.13
7.11
7.09
7.07
7.04
6.99
6.99
1.59
0.00
OH
S
N
3ak
4.01
2.97
1.04
1.00
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
0.0
f1 (ppm)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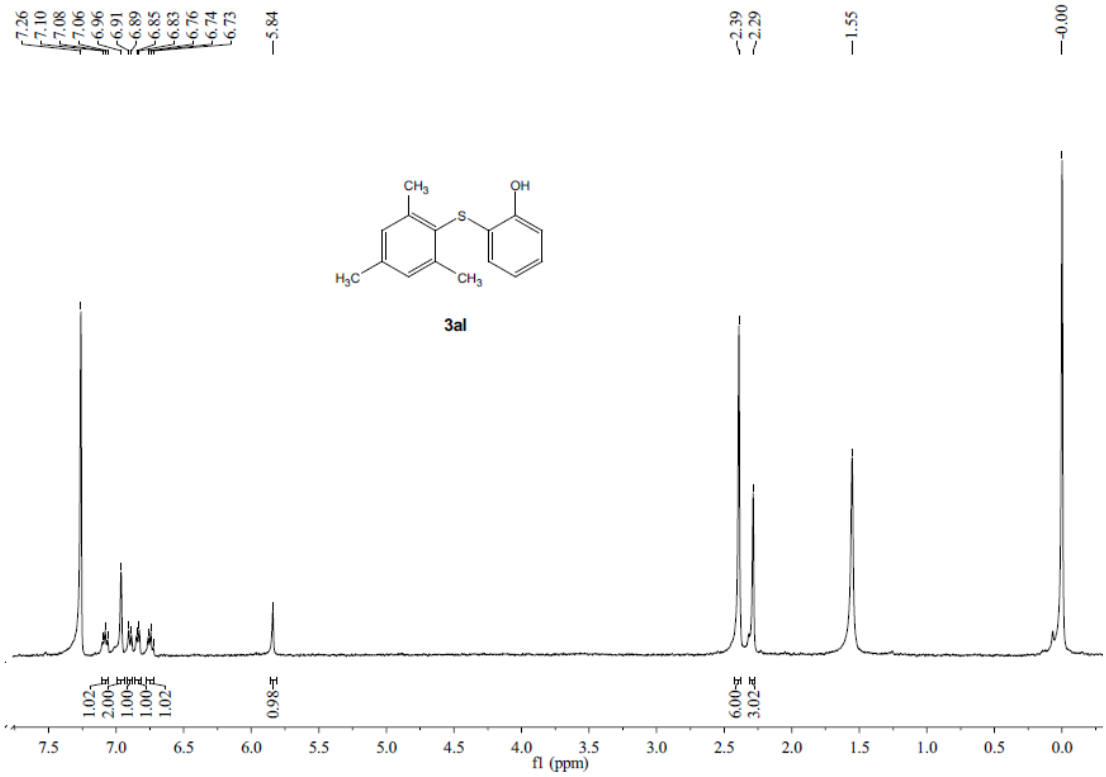
143.54
137.12
133.25
132.80
132.58
126.68
126.27
121.82
118.52
116.24
77.42
77.10
76.78
OH
S
N
3ak
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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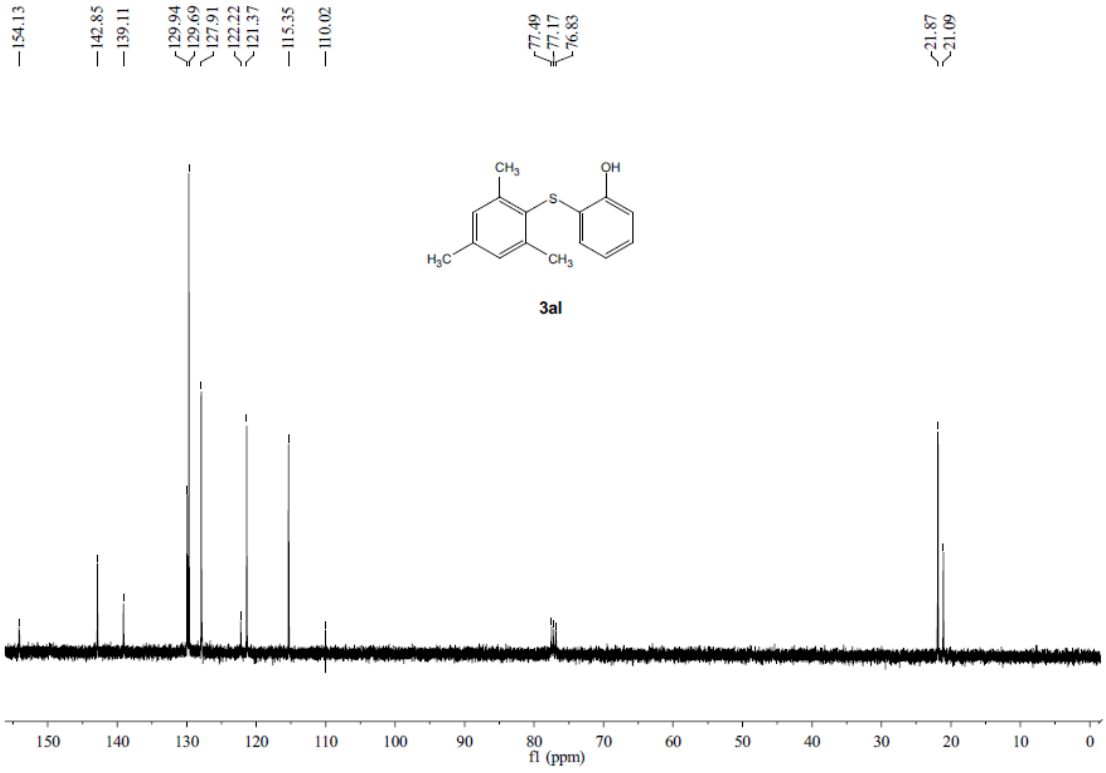
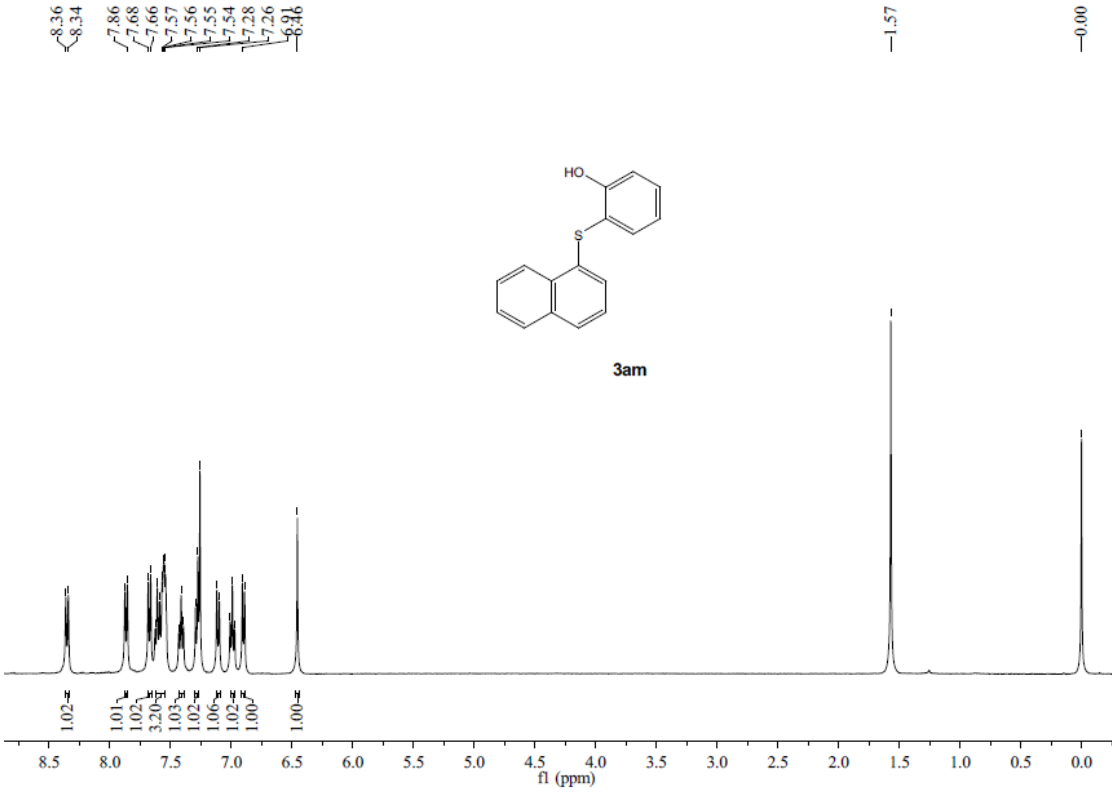
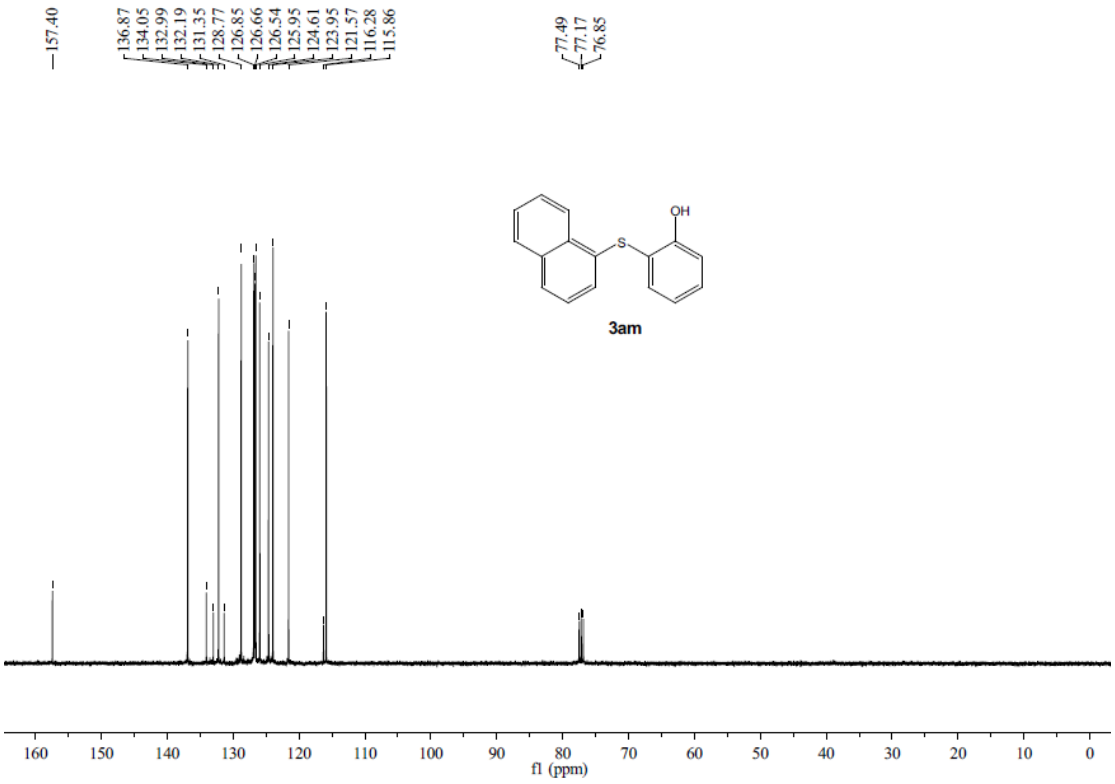
7.10
7.08
7.06
6.96
6.91
6.89
6.85
6.83
6.76
6.74
6.73
5.84
2.39
2.29
1.55
0.00
CH3
OH
S
H3C
CH3
3al
1.02
2.00
1.00
1.00
1.02
0.98
6.00
3.02
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


154.13
142.85
139.11
129.94
129.69
127.91
122.22
121.37
115.35
110.02
77.49
77.17
76.83
21.87
21.09
CH3
OH
S
H3C
CH3
3al
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.36
8.34
7.86
7.68
7.66
7.57
7.56
7.55
7.54
7.28
7.26
6.91
6.46
1.57
0.00
HO
S
3am
1.02
1.01
1.02
3.20
1.03
1.02
1.06
1.02
1.00
1.00
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
0.0
f1 (ppm)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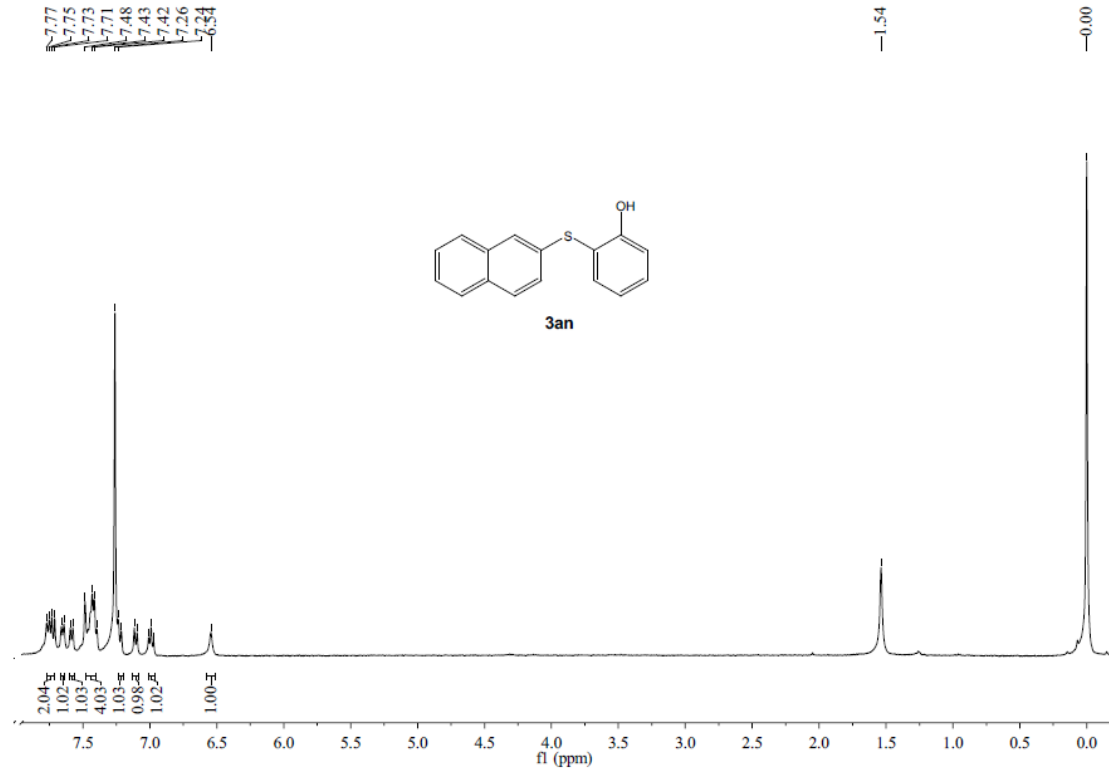
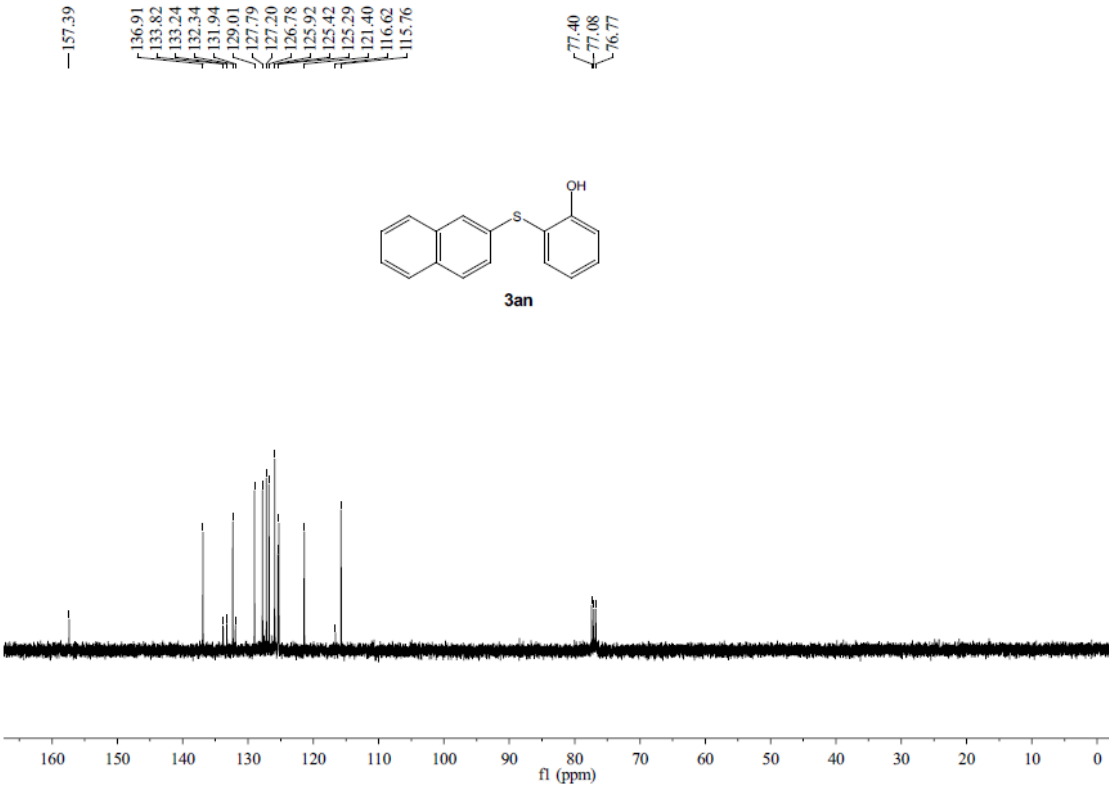
136.87
134.05
132.99
132.19
131.35
128.77
126.85
126.66
126.54
125.95
124.61
123.95
121.57
116.28
115.86
77.49
77.17
76.85
OH
S
3am
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.77
7.75
7.73
7.71
7.48
7.43
7.42
7.26
6.54
1.54
0.00
OH
S
3an
2.04
1.02
1.03
4.03
1.03
0.98
1.02
1.00
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
0.0
f1 (ppm)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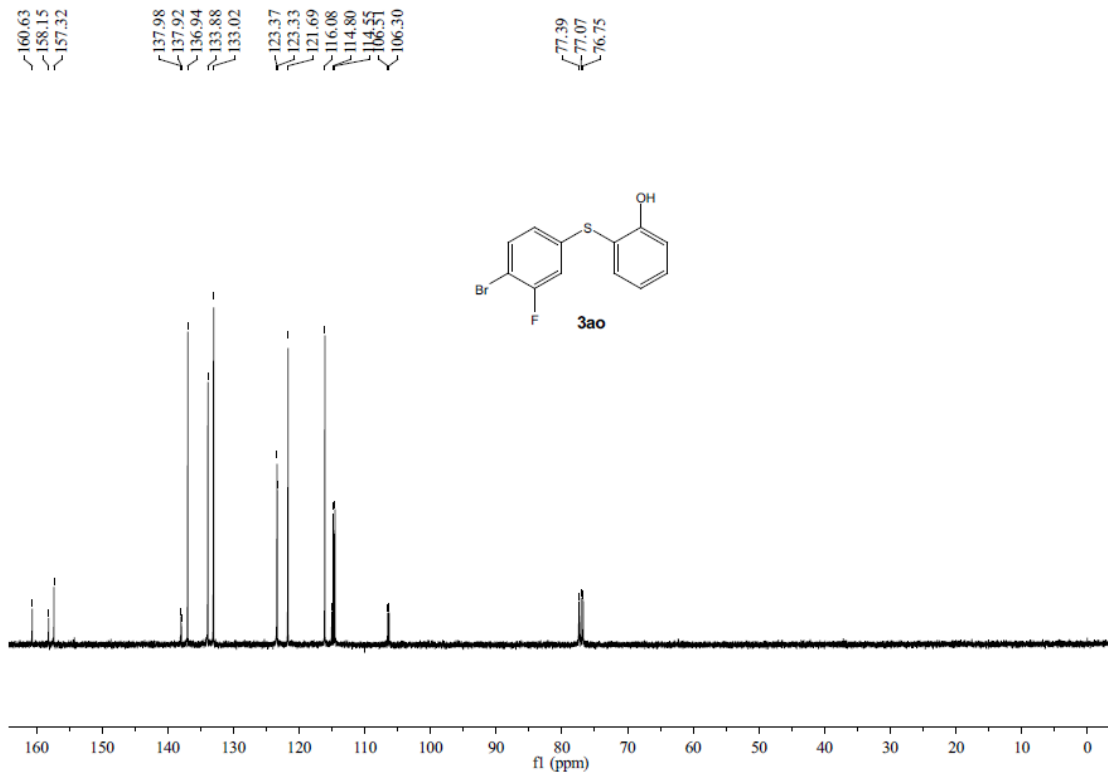
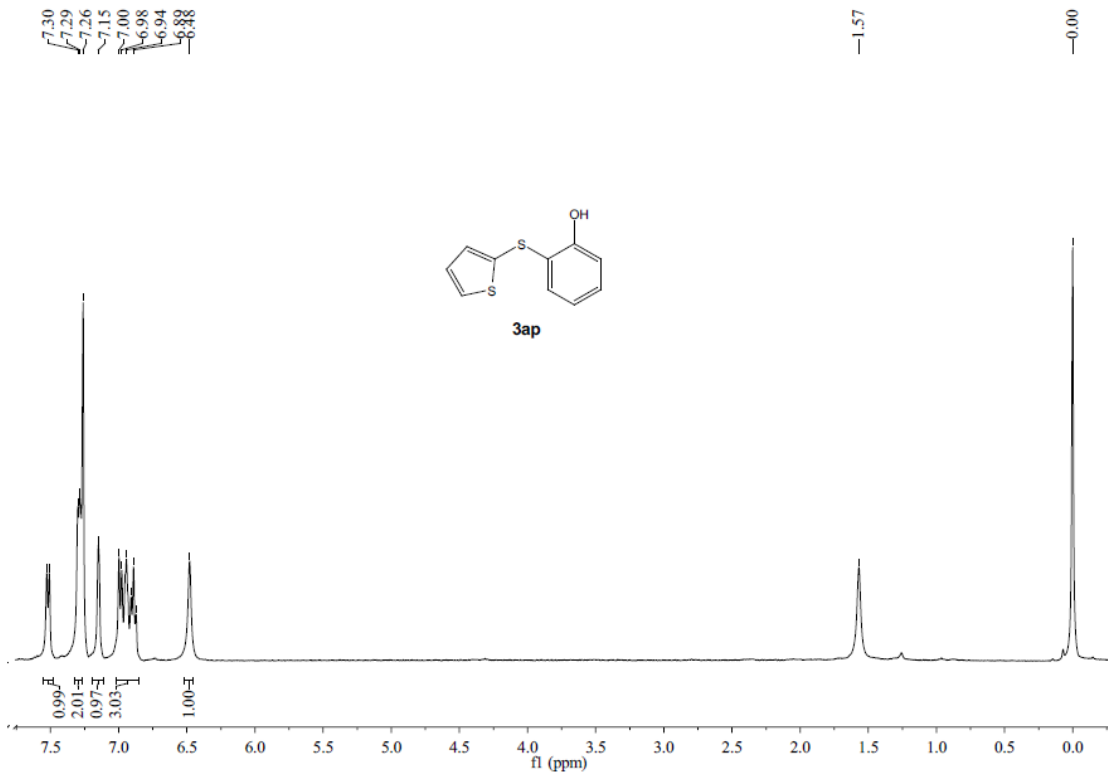
136.91
133.82
133.24
132.34
131.94
129.01
127.79
127.20
126.78
125.92
125.42
125.29
121.40
116.62
115.76
77.40
77.08
76.77
OH
S
3an
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.43
7.41
7.39
7.26
7.11
7.00
6.77
6.76
6.74
6.33
1.55
0.00
OH
S
Br
F
3ao
1.02
2.10
1.03
0.98
2.05
1.00
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
0.0
f1 (ppm)


160.63
158.15
157.32
137.98
137.92
136.94
133.88
133.02
123.37
123.33
121.69
116.08
114.80
114.55
106.51
106.30
77.39
77.07
76.75
OH
S
Br
F
3ao
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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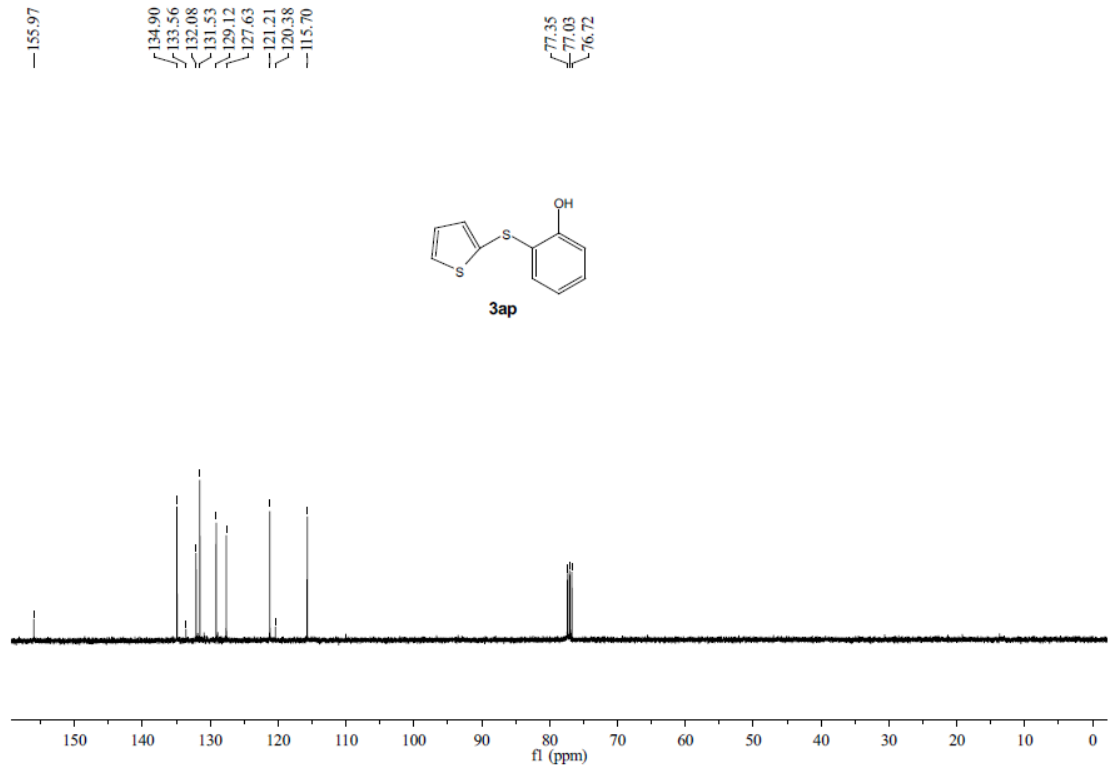
7.29
7.26
7.15
7.00
6.98
6.94
6.89
6.88
1.57
0.00
OH
S
S
3ap
0.99
2.01
0.97
3.03
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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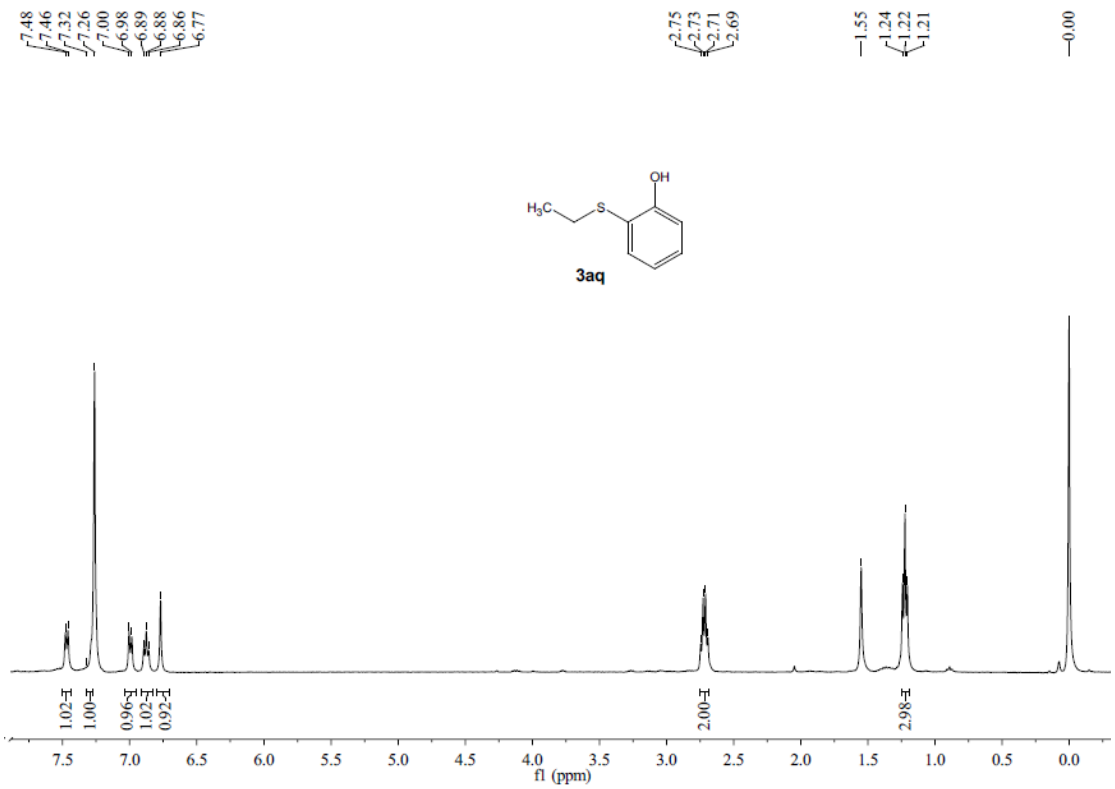
134.90
133.56
132.08
131.53
129.12
127.63
121.21
120.38
115.70
77.35
77.03
76.72
OH
S
S
3ap
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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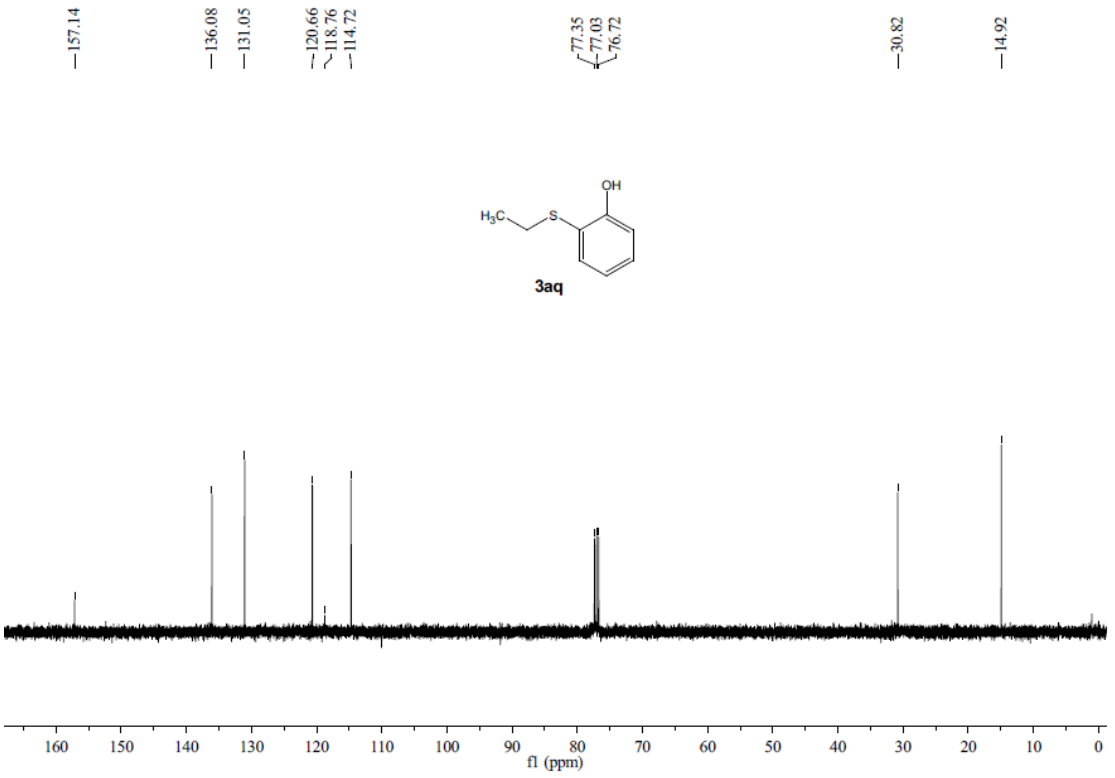
7.46
7.32
7.26
7.00
6.98
6.89
6.88
6.86
6.77
2.75
2.73
2.71
2.69
1.55
1.24
1.22
1.21
0.00
OH
H3C
S
3aq
1.02
1.00
0.96
1.02
0.92
2.00
2.98
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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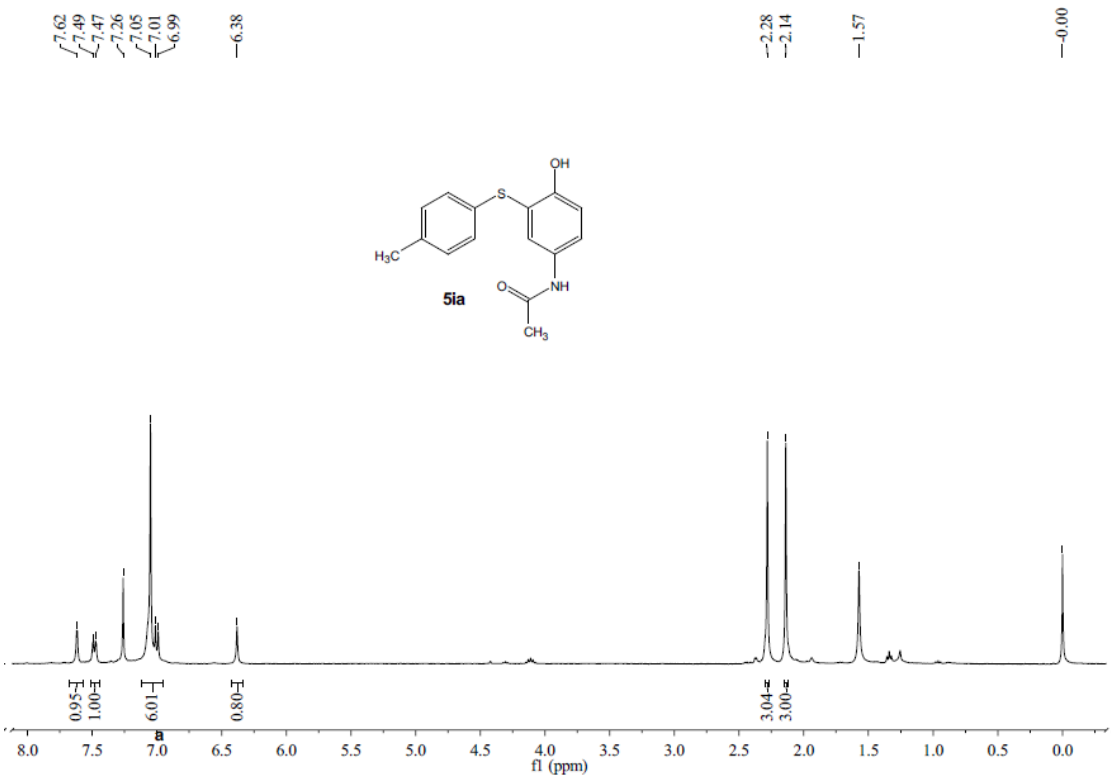
136.08
131.05
120.66
118.76
114.72
77.35
77.03
76.72
30.82
14.92
OH
H3C
S
3aq
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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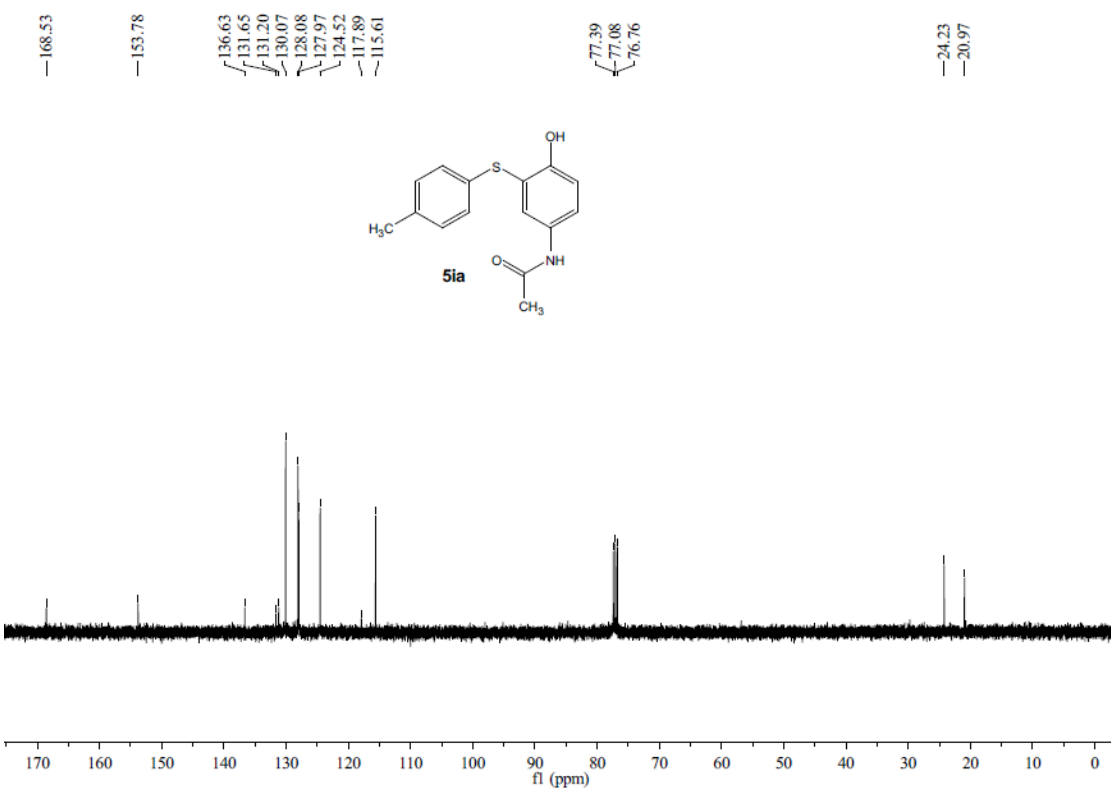
7.49
7.47
7.26
7.05
7.01
6.99
6.38
2.28
2.14
1.57
0.00
OH
S
H3C
NH
O
CH3
5ia
0.95
1.00
6.01
0.80
3.04
3.00
a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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153.78
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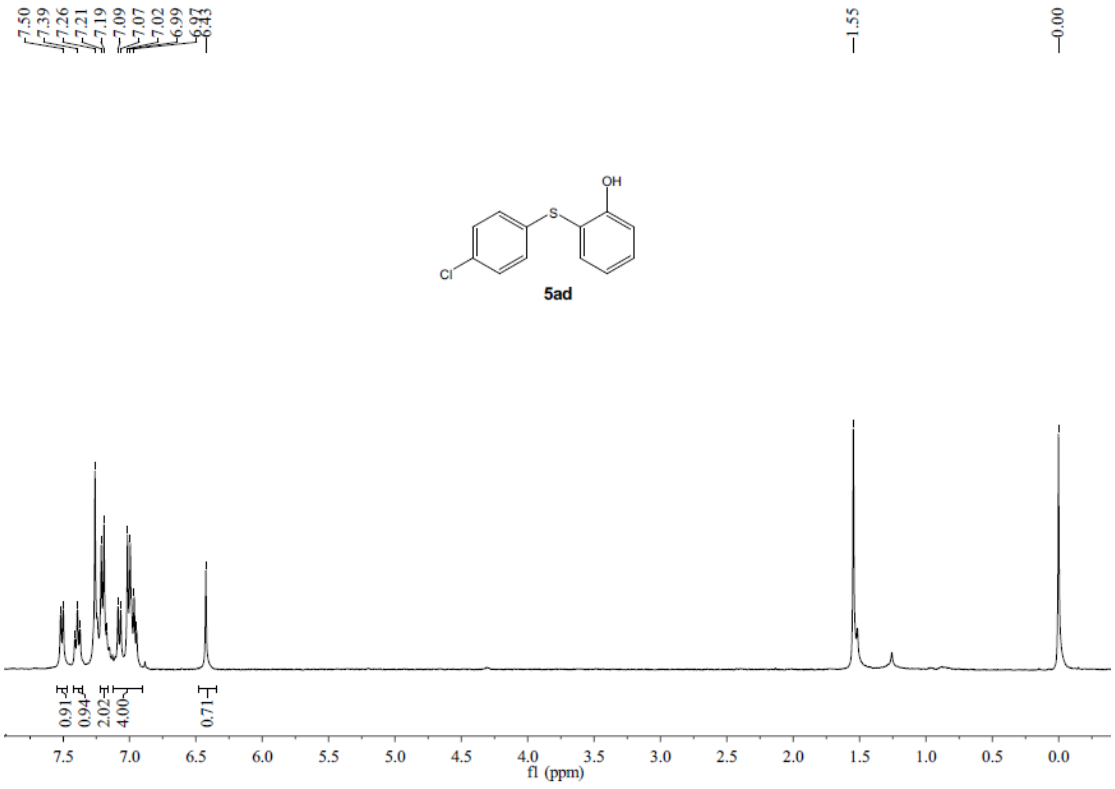
131.65
131.20
130.07
128.08
127.97
124.52
117.89
115.61
77.39
77.08
76.76
24.23
20.97
OH
S
H3C
NH
O
CH3
5ia
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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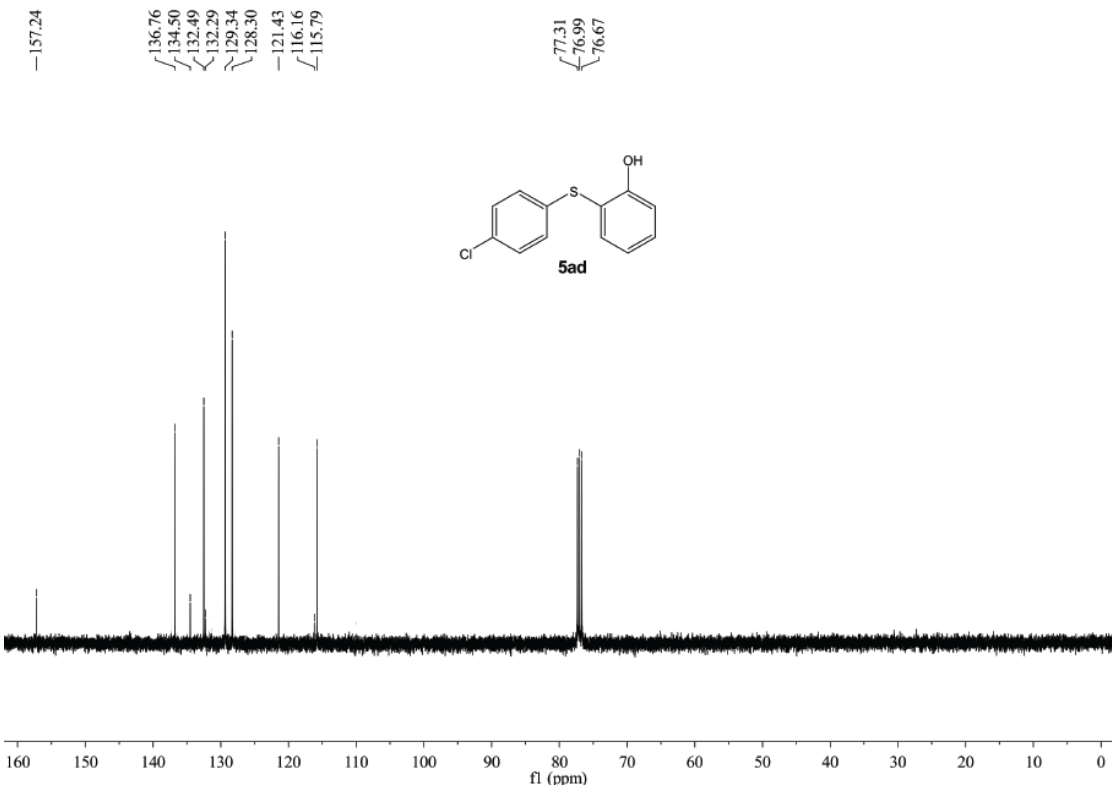
7.39
7.26
7.21
7.19
7.09
7.07
7.02
6.99
6.97
6.43
1.55
0.00
OH
S
Cl
5ad
0.91
0.94
2.02
4.00
0.71
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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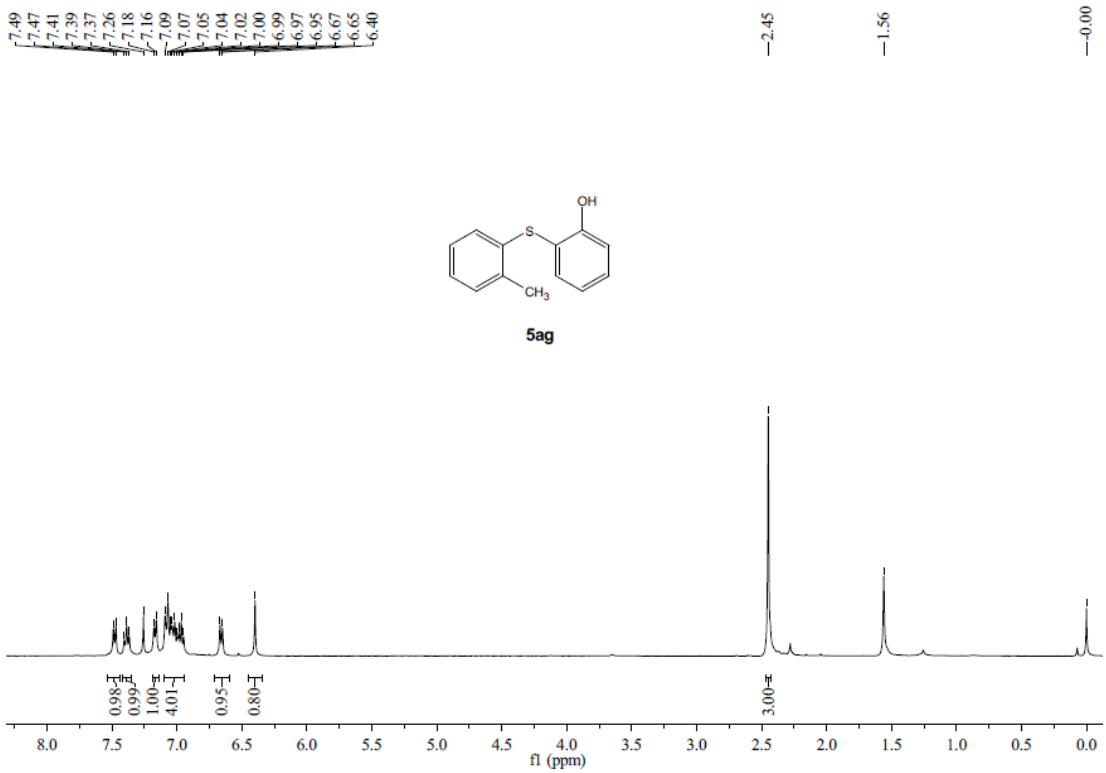
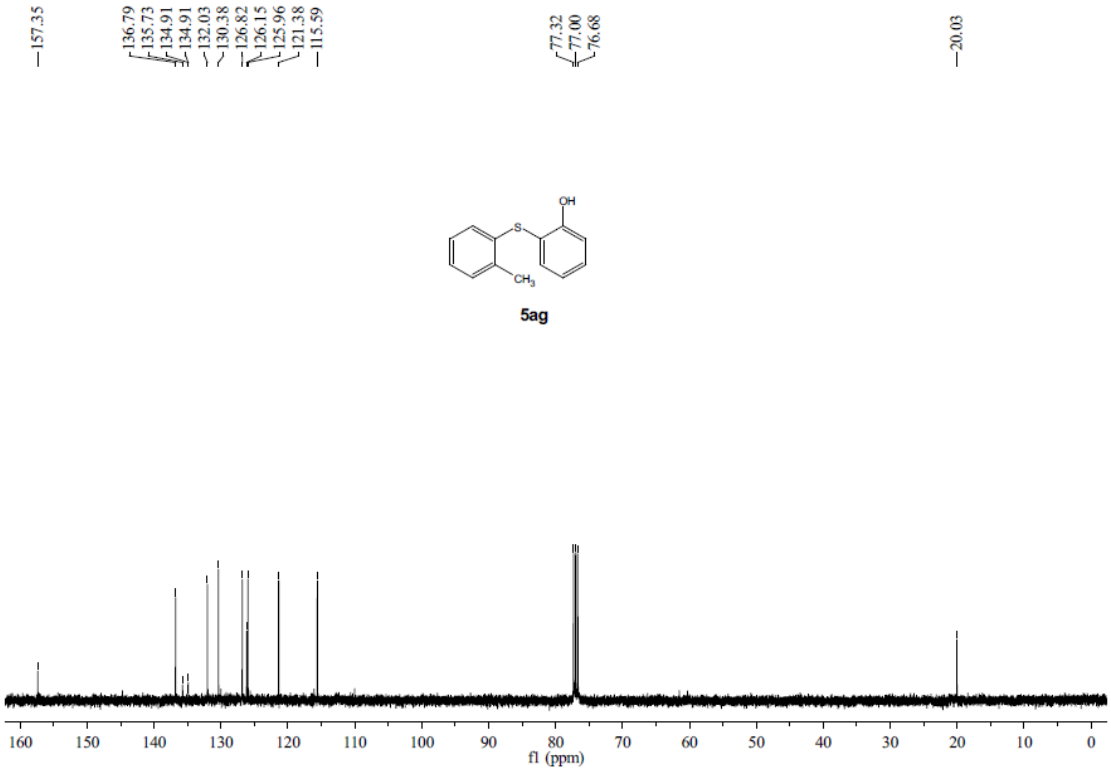
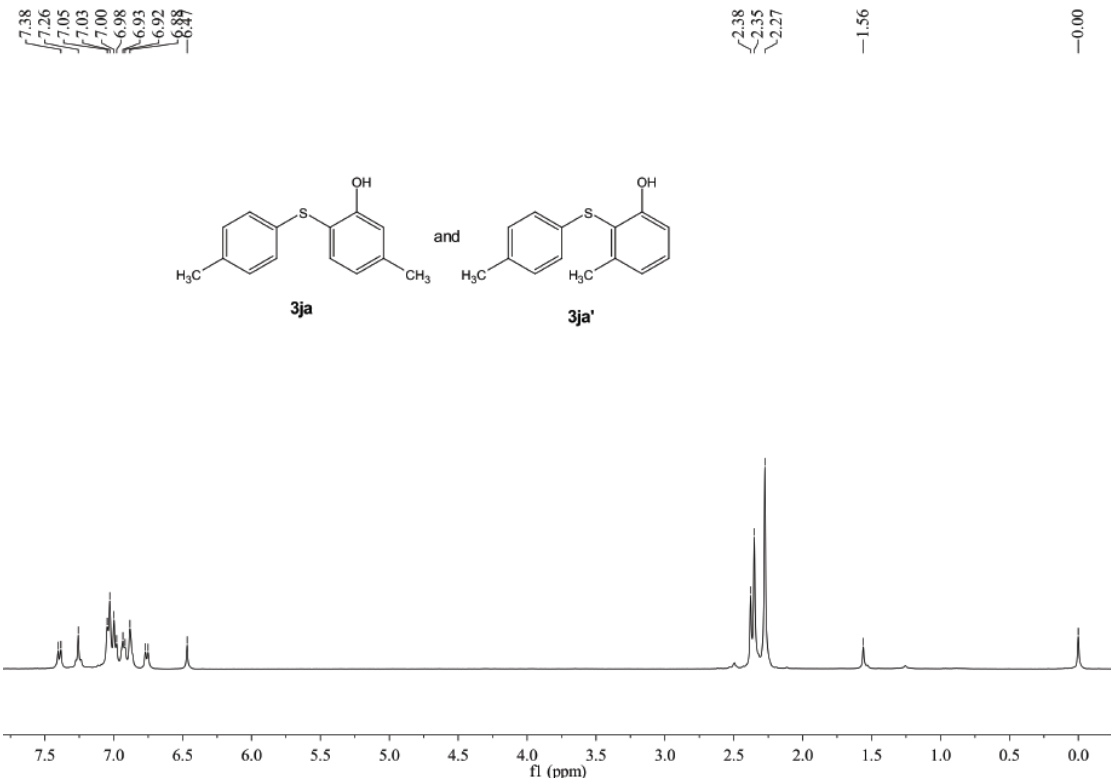
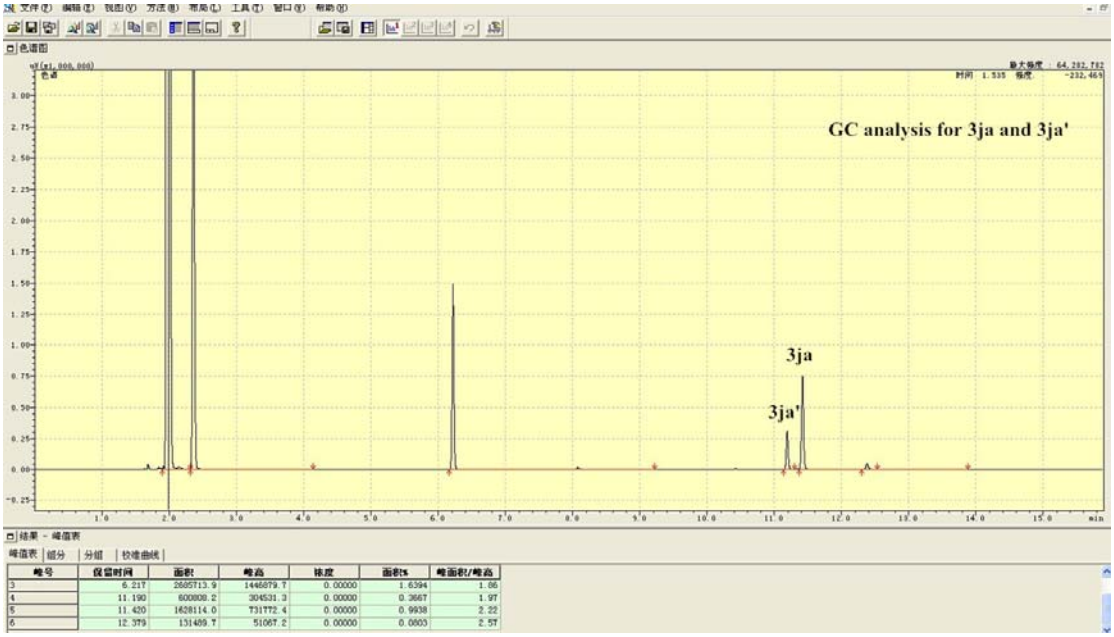
132.49
132.29
129.34
128.30
121.43
116.16
115.79
77.31
76.99
76.67
OH
S
Cl
5ad
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.49
7.47
7.41
7.39
7.37
7.26
7.18
7.16
7.09
7.07
7.05
7.04
7.02
7.00
6.99
6.97
6.95
6.67
6.65
6.40
2.45
1.56
0.00
OH
S
CH3
5ag
0.98
0.99
1.00
4.01
0.95
0.80
3.00
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
0.0
f1 (ppm)


157.35
136.79
135.73
134.91
134.91
132.03
130.38
126.82
126.15
125.96
121.38
115.59
77.32
77.00
76.68
20.03
OH
S
CH3
5ag
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.38
7.26
7.05
7.03
7.00
6.98
6.93
6.92
6.88
6.87
2.38
2.35
2.27
1.56
0.00
OH
S
H3C
CH3
3ja
and
OH
S
H3C
H3C
3ja'
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
0.0
f1 (ppm)


GC analysis for 3ja and 3ja'
3ja
3ja'