Electronic Supporting Information for

Aerobic oxysulfonylation of alkenes using thiophenols: An efficient one-pot route to β-ketosulfones

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i. General information: Reagents were obtained from commercial suppliers, and used without further purification. Organic solutions were concentrated using a Buchi rotary evaporator. Column chromatography was carried out over silica gel (Merck 100–200 mesh) and TLC was performed using silica gel GF254 (Merck) plates. ^{1}H NMR spectra were recorded on a Bruker AVII 400 spectrometer in $CDCl_3$ using TMS as internal reference with chemical shift value being reported in ppm. All coupling constants (*J*) are reported in hertz (Hz). ^{13}C NMR spectra were recorded on the same instrument at 100 MHz in $CDCl_3$ and TMS was used as internal reference. Mass (EI) spectra were recorded on a JEOL D-300 mass spectrometer. Elemental analyses were carried out in a Coleman automatic analyzer.

ii. General procedure

a. General procedure for the one-pot synthesis of β-ketosulfones 3a-3t

A mixture of alkene **1** (0.25 mmol), thiophenol/thiol **2** (0.25 mmol), $AgNO_3$ (20 mol %), $K_2S_2O_8$ (0.75 mmol) and DMF (3 mL) was stirred at rt in an open flask for 18-22 h (Table 2). After completion of the reaction (monitored by TLC), the mixture was extracted with EtOAc (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using a mixture of EtOAc-*n*-hexane (1:4) as eluent to afford an analytically pure sample of β-keto sulfones **3** (Table 2).

b. Typical procedure for radical trapping experiment

A mixture of styrene **1a** (0.25 mmol), thiophenol **2a** (0.25 mmol), $AgNO_3$ (20 mol%), and TEMPO (0.25 mmol) in DMF (3 mL) was stirred at rt in an open flask for 4 h. After the reaction, the solution was concentrated in vacuum, no desired product was detected.

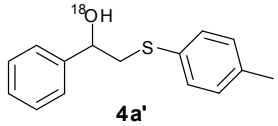
c. Typical procedure for studying the role of air

A mixture of styrene **1a** (0.25 mmol), thiophenol **2a** (0.25 mmol), and $AgNO_3$ (20 mol%) in DMF (3 mL) was stirred at rt under nitrogen atmosphere for 4 h. After completion of the reaction (monitored by TLC), the mixture was extracted with EtOAc (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using a mixture of EtOAc-*n*-hexane (1:4) as eluent to afford β-hydroxysulfide **4a** in traces (checked by TLC) and styrene was recovered.

d. Typical procedure for ^{18}O labeling experiments

A mixture of styrene **1a** (0.25 mmol), thiophenol **2a** (0.25 mmol), and $AgNO_3$ (20 mol %) in DMF (3 mL) was stirred at rt under $^{18}O_2/N_2$ atmosphere for 4 h. After completion of the reaction (monitored by TLC), the mixture was extracted with EtOAc (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered and concentrated under reduced pressure. The resulting crude product was purified by silica gel column

chromatography using a mixture of EtOAc-*n*-hexane (1:4) as eluent to afford an analytically pure sample of β-hydroxysulfide **4a'** (yield 88%).



4a'

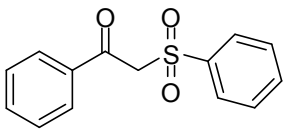
e. Typical procedure for probing the intermediate

A mixture of 1-phenyl-2-tosylethanol (0.25 mmol) and $K_2S_2O_8$ (0.75 mmol) in DMF (3 mL) was stirred at rt in an open flask for 16 h. After completion of the reaction (monitored by TLC), the mixture was extracted with EtOAc (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using a mixture of EtOA-*n*hexane (1:4) as eluent to afford β-ketosulfone **3a** in 95% yield.

f. General procedure for the synthesis of β-hydroxysulfides 4

A mixture of alkene **1** (0.25 mmol), thiophenol/thiol **2** (0.25 mmol), $AgNO_3$ (20 mol %), and DMF (3 mL) was stirred at rt in an open flask for 2-6 h (Table 3). After completion of the reaction (monitored by TLC), the mixture was extracted with EtOAc (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using a mixture of EtOAc-*n*-hexane (1:4) as eluent to afford an analytically pure sample of β-hydroxysulfides **4** (Table 3).

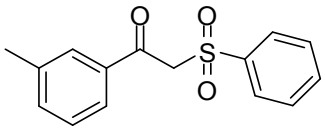
iii. Spectroscopic and analytical data for compounds 3 and 4



1-phenyl-2-(phenylsulfonyl)ethanone (3a)[1]

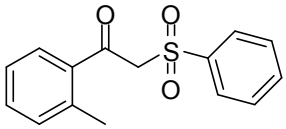
Solid; 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.90 (m, 4H), 7.64-7.57 (m, 2H), 7.53 (t, J = 7.6 Hz, 2H), 7.51 (t, J = 7.6 Hz, 2H), 4.78 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.98,

138.83, 135.84, 134.36, 134.28, 129.30, 129.25, 128.84, 128.63, 63.52. EIMS (*m*/*z*): 260 (M^+). Anal. Calcd for $C_{14}H_{12}O_3S$: C, 64.60; H, 4.65; S, 12.32. Found: C, 64.44; H, 4.95; S, 12.06.



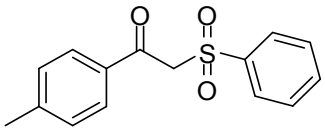
2-(phenylsulfonyl)-1-*m*-tolylethanone (3b)[2]

Solid; 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, J = 8.2, 1.2 Hz, 2H), 7.72 (d, J = 9.4 Hz, 2H), 7.69-7.63 (m, 1H), 7.52 (t, J = 7.6 Hz, 2H), 7.45 (d, J = 7.6 Hz, 1H), 7.31 (t, J = 7.4 Hz, 1H), 4.75 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.10, 138.90, 138.76, 135.82, 135.24, 134.21, 129.68, 129.17, 128.72, 128.65, 126.56, 63.50, 21.32. EIMS (*m*/*z*): 274 (M^+). Anal. Calcd for $C_{15}H_{14}O_3S$: C, 65.67; H, 5.14; S, 11.69. Found: C, 65.57; H, 5.49; S, 11.53.



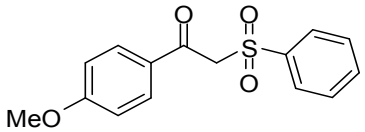
2-(phenylsulfonyl)-1-*o*-tolylethanone (3c)[2]

Solid; 88% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.2 Hz, 2H), 7.74 (d, J = 7.4 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.41 (t, J = 7.8 Hz, 1H), 7.28-7.20 (m, 2H), 4.73 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.40, 140.09, 139.05, 135.78, 134.15, 132.82, 132.39, 130.32, 129.20, 128.49, 125.98, 65.52, 21.51. EIMS (*m*/*z*): 274 (M^+). Anal. Calcd for $C_{15}H_{14}O_3S$: C, 65.67; H, 5.14; S, 11.69. Found: C, 65.98; H, 5.02; S, 11.42.



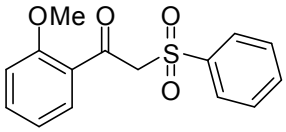
2-(phenylsulfonyl)-1-*p*-tolylethanone (3d)[3]

Solid; 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 7.2 Hz, 2H), 7.82 (d, J = 8.2 Hz, 2H), 7.60 (t, J = 7.2 Hz, 1H), 7.56 (t, J = 7.8 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 4.79 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.67, 145.75, 138.90, 134.35, 133.49, 129.77, 129.57, 129.35, 128.72, 63.62, 21.94. EIMS (*m*/*z*): 274 (M^+). Anal. Calcd for $C_{15}H_{14}O_3S$: C, 65.67; H, 5.14; S, 11.69. Found: C, 65.80; H, 5.33; S, 11.49.



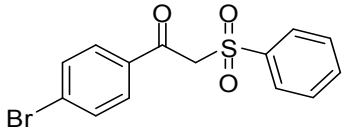
1-(4-methoxyphenyl)-2-(phenylsulfonyl)ethanone (3e)[4]

Solid; 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, J = 16.6, 8.4 Hz, 4H), 7.67 (t, J = 7.4 Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 4.75 (s, 2H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.26, 164.70, 138.89, 134.32, 131.95, 129.27, 128.99, 128.63, 114.25, 63.53, 55.76. EIMS (*m*/*z*): 290 (M^+). Anal. Calcd for $C_{15}H_{14}O_4S$: C, 62.05; H, 4.86; S, 11.04. Found: C, 62.13; H, 5.03; S, 10.96.



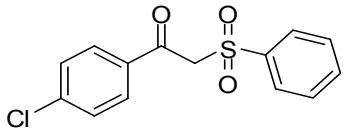
1-(2-methoxyphenyl)-2-(phenylsulfonyl)ethanone (3f)[5]

Solid; 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.6 Hz, 2H), 7.64 (dd, J = 7.6, 2.0 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.50-7.41 (m, 3H), 6.91 (t, J = 7.4 Hz, 1H), 6.84 (d, J = 8.4 Hz, 1H), 4.95 (s, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.09, 159.12, 139.75, 135.45, 133.91, 131.47, 129.07, 128.71, 126.34, 121.17, 111.87, 67.51, 55.83. EIMS (*m*/*z*): 290 (M^+). Anal. Calcd for $C_{15}H_{14}O_4S$: C, 62.05; H, 4.86; S, 11.04. Found: C, 62.01; H, 4.97; S, 11.26.



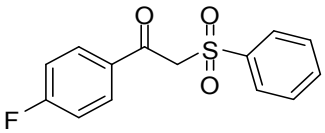
1-(4-bromophenyl)-2-(phenylsulfonyl)ethanone (3g)[1]

Solid; 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.2 Hz, 2H), 7.84 (d, J = 8.6 Hz, 2H), 7.73 (t, J = 7.6 Hz, 1H), 7.65 (d, J = 8.5 Hz, 2H), 7.53 (t, J = 7.6 Hz, 2H), 4.70 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.23, 138.70, 134.69, 134.52, 132.45, 130.97, 130.21, 129.40, 128.71, 63.75. EIMS (*m*/*z*): 337, 339 (M^+, M^+ + 2). Anal. Calcd for $C_{14}H_{11}BrO_3S$: C, 49.57; H, 3.27; S, 9.45. Found: C, 49.42; H, 3.18; S, 9.76.



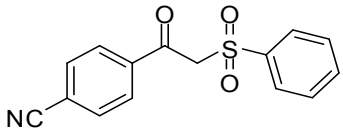
1-(4-chlorophenyl)-2-(phenylsulfonyl)ethanone (3h)[4]

Solid; 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.88 (m, 4H), 7.70 (t, J = 7.5 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 4.76 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.97, 141.25, 138.68, 134.54, 134.13, 130.89, 129.46, 129.35, 128.70, 63.75. EIMS (*m*/*z*): 294, 296 (M^+, M^+ + 2). Anal. Calcd for $C_{14}H_{11}ClO_3S$: C, 57.05; H, 3.76; S, 10.88. Found: C, 57.23; H, 3.44; S, 10.77.



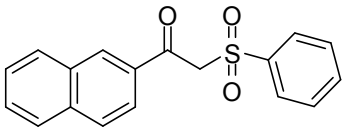
1-(4-fluorophenyl)-2-(phenylsulfonyl)ethanone (3i)[2]

Solid; 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, J = 8.6, 5.4 Hz, 2H), 7.90 (d, J = 7.4 Hz, 2H), 7.76 (t, J = 7.6 Hz, 1H), 7.61 (t, J = 7.7 Hz, 2H), 7.23 (t, J = 7.6 Hz, 2H), 4.78 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.43, 167.79, 165.30, 138.76, 134.39, 132.30, 132.19, 129.30, 128.53, 116.24, 116.00, 63.62. EIMS (*m*/*z*): 278 (M^+). Anal. Calcd for $C_{14}H_{11}FO_3S$: C, 60.42; H, 3.98; S, 11.52. Found: C, 60.55; H, 4.11; S, 11.35.



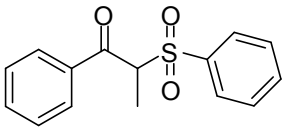
4-(2-(phenylsulfonyl)acetyl)benzonitrile (3j)[2]

Solid; 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 7.2 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.69 (t, J = 7.4 Hz, 1H), 7.61 (t, J = 7.6 Hz, 2H), 4.78 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.06, 138.53, 138.49, 134.53, 132.68, 129.70, 129.42, 128.53, 117.69, 117.57, 63.76. EIMS (*m*/*z*): 285 (M^+). Anal. Calcd for $C_{15}H_{11}NO_3S$: C, 63.14; H, 3.89; N, 4.91; S, 11.24. Found: C, 63.01; H, 3.98; N, 4.99; S, 11.59.



1-(naphthalen-2-yl)-2-(phenylsulfonyl)ethanone (3k)[2]

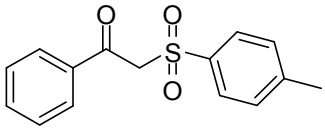
Solid; 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.01-7.90 (m, 6H), 7.62 (t, J = 7.4 Hz, 2H), 7.60-7.55 (m, 3H), 4.82 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.82, 138.85, 136.14, 134.21, 133.12, 132.36, 132.13, 129.98, 129.46, 129.26, 128.89, 128.63, 127.78, 127.20, 123.99, 63.72. EIMS (*m*/*z*): 310 (M^+). Anal. Calcd for $C_{18}H_{14}O_3S$: C, 69.66; H, 4.55; S, 10.33. Found: C, 69.80; H, 4.22; S, 10.54.



1-phenyl-2-(phenylsulfonyl)propan-1-one (3l)[6]

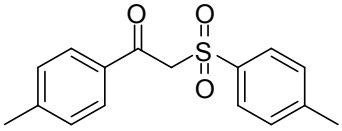
Solid; 84% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 7.85-7.78 (m, 2H), 7.64 (tt, J = 7.2, 1.4 Hz, 1H), 7.52 (tt, J = 7.6, 1.4 Hz, 1H), 7.46 (tt, J = 8.2, 1.4 Hz, 2H), 7.40 (tt, J = 7.6, 1.8 Hz, 2H), 5.25 (q, J = 2.6 Hz, 1H), 1.56 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.69, 136.33, 136.19, 134.37, 134.22, 129.96, 129.30, 129.10, 128.90, 65.17, 13.40. EIMS

(*m*/*z*): 274 (M^+). Anal. Calcd for $C_{15}H_{14}O_3S$: C, 65.67; H, 5.14; S, 11.69. Found: C, 65.58; H, 5.38; S, 11.56.



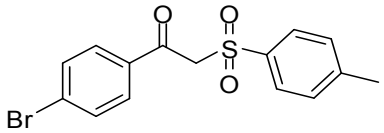
1-phenyl-2-tosylethanone (3m)[1]

Solid; 94% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 7.6 Hz, 2H), 7.83 (t, J = 8.6, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 4.67 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.30, 145.51, 135.89, 135.84, 134.48, 129.93, 129.42, 128.98, 128.75, 63.90, 21.82. EIMS (*m*/*z*): 274 (M^+). Anal. Calcd for $C_{15}H_{14}O_3S$: C, 65.67; H, 5.14; S, 11.69. Found: C, 65.83; H, 5.32; S, 11.51.



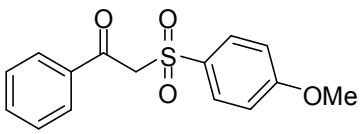
1-*p*-tolyl-2-tosylethanone (3n)[7]

Solid; 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.30-7.24 (m, 2H), 7.22-7.19 (m, 2H), 4.69 (s, 2H), 2.45 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.64, 145.40, 145.14, 136.09, 133.44, 129.68, 129.40, 129.37, 128.49, 63.55, 21.58, 21.51. EIMS (*m*/*z*): 288 (M^+); Anal. Calcd for $C_{16}H_{16}O_3S$: C, 66.64; H, 5.59; S, 11.12; Found: C, 66.81; H, 5.39; S, 11.36.



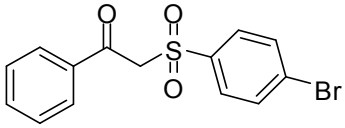
1-(4-bromophenyl)-2-tosylethanone (3o)[2]

Solid; 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, J = 6.8, 2.0 Hz, 2H), 7.74 (d, J = 8.2 Hz, 2H), 7.67 (d, J = 8.6 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 4.63 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.30, 145.60, 135.61, 134.53, 132.27, 130.83, 129.95, 129.90, 128.57, 63.79, 21.74. EIMS (*m*/*z*): 351, 353 (M^+, M^+ + 2). Anal. Calcd for $C_{15}H_{13}BrO_3S$: C, 51.00; H, 3.71; S, 9.08. Found: C, 51.14; H, 3.40; S, 9.19.



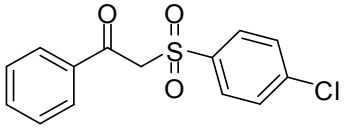
2-(4-methoxyphenylsulfonyl)-1-phenylethanone (3p)[4]

Solid; 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.2 Hz, 2H), 7.80 (d, J = 9.0 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.8 Hz, 2H), 7.10 (d, J = 9.0 Hz, 2H), 4.69 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.44, 164.26, 135.95, 134.49, 130.96, 130.38, 129.43, 128.92, 114.56, 63.89, 55.87. EIMS (*m*/*z*): 290 (M^+). Anal. Calcd for $C_{15}H_{14}O_4S$: C, 62.05; H, 4.86; S, 11.04. Found: C, 61.96; H, 4.56; S, 11.40.



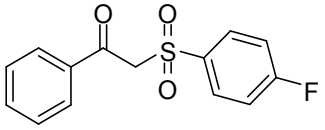
2-(4-bromophenylsulfonyl)-1-phenylethanone (3q)[1]

Solid; 79% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, J = 8.2, 1.2 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 4.79 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.01, 137.79, 135.64, 134.61, 132.60, 130.35, 129.94, 129.30, 129.04, 63.54. EIMS (*m*/*z*): 337, 339 (M^+, M^+ + 2). Anal. Calcd for $C_{14}H_{11}BrO_3S$: C, 49.57; H, 3.27; S, 9.45. Found: C, 49.71; H, 3.40; S, 9.76.



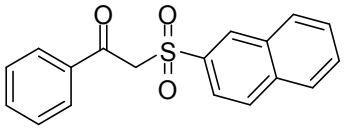
2-(4-chlorophenylsulfonyl)-1-phenylethanone (3r)[2]

Solid; 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 7.6 Hz, 2H), 7.84 (d, J = 8.4 Hz, 2H), 7.63 (t, J = 7.2 Hz, 1H), 7.49-7.43 (m, 4H), 4.78 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.10, 141.25, 137.26, 135.69, 134.62, 130.33, 129.69, 129.35, 129.08, 63.51. EIMS (*m*/*z*): 294, 296 (M^+, M^+ + 2). Anal. Calcd for $C_{14}H_{11}ClO_3S$: C, 57.05; H, 3.76; S, 10.88. Found: C, 57.17; H, 3.59; S, 10.56.



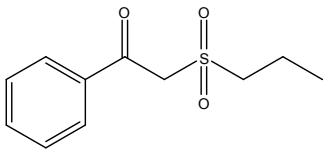
2-(4-fluorophenylsulfonyl)-1-phenylethanone (3s)[4]

Solid; 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.89 (m, 4H), 7.61-7.58 (m, 1H), 7.50 (t, J = 7.8 Hz, 2H), 7.24 (t, J = 8.2 Hz, 2H), 4.77 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.25, 167.60, 164.92, 135.78, 134.65, 131.80, 131.73, 129.40, 129.06, 116.87, 116.52, 63.58. EIMS (*m*/*z*): 278 (M^+). Anal. Calcd for $C_{14}H_{11}FO_3S$: C, 60.42; H, 3.98; S, 11.52. Found: C, 60.29; H, 3.70; S, 11.59.



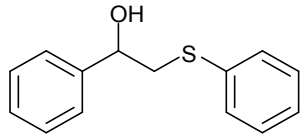
2-(naphthalen-2-ylsulfonyl)-1-phenylethanone (3t)[1]

Solid; 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 1.4 Hz, 1H), 7.94-7.81 (m, 6H), 7.68 (t, J = 7.2 Hz, 1H), 7.66-7.57 (m, 2H), 7.50 (t, J = 7.8 Hz, 2H) 4.80 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.11, 135.87, 135.79, 135.63, 134.42, 132.08, 130.77, 129.70, 129.69, 129.61, 129.44, 128.90, 128.17, 127.84, 123.11, 63.69. EIMS (*m*/*z*): 310 (M^+). Anal. Calcd for $C_{18}H_{14}O_3S$: C, 69.66; H, 4.55; S, 10.33. Found: C, 69.81; H, 4.62; S, 10.07.



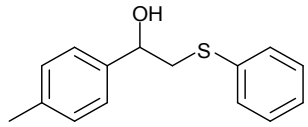
1-phenyl-2-(propylsulfonyl)ethanone (3u)

Liquid; 84% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.93-7.95 (m, 2 H), 7.53-7.60 (m, 1 H), 7.36-7.47 (m, 2 H), 4.49 (s, 2 H), 3.15-3.19 (m, 2 H), 1.82-1.90 (m, 2 H), 1.02-1.05 (t, J = 7.4 Hz, 3 H), ^{13}C NMR (100 MHz, $CDCl_3$) δ: 189.2, 135.5, 134.7, 129.2, 129.0, 61.2, 52.10, 15.93, 13.01. EIMS (*m*/*z*): 226 (M^+). Anal. Calcd for $C_{11}H_{14}O_3S$: C, 58.38; H, 6.24; S, 14.17. Found: C, 58.62; H, 6.06; S, 14.29.



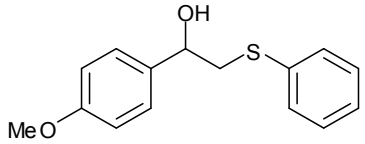
1-phenyl-2-(phenylthio)ethanol (4a)[8]

Oil; 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.41 (m, 2 H), 7.37-7.29 (m, 8 H), 4.75 (dd, J = 9.2, 3.1 Hz, 1 H), 3.35 (dd, J = 13.6, 3.6 Hz, 1 H), 3.12-3.10 (m, 1 H), 2.95 (br s, 1 H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.12, 134.93, 130.23, 129.14, 128.49, 128.01, 126.72, 125.78, 71.65, 44.04. EIMS (*m*/*z*): 230 (M^+). Anal. Calcd for $C_{14}H_{14}OS$: C, 73.01; H, 6.13; S, 6.95. Found: C, 73.13; H, 5.98; S, 7.33.



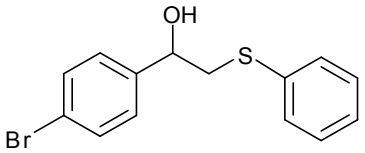
2-(phenylthio)-1-p-tolylethanol (4b)[9]

Pale yellow oil; 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, J = 8.7 Hz, 2H), 7.34-7.19 (m, 5H), 7.09 (d, J = 8.5 Hz, 2H), 4.65 (d, J = 9.6 Hz, 1H), 3.30 (dd, J = 3.6, 14.2 Hz, 1H), 3.10-3.00 (m, 1H), 2.69 (d, J = 2.4 Hz,1H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.14, 137.73, 134.85, 130.32, 129.14, 128.76, 125.82, 125.55, 71.53, 44.02, 21.39. EIMS (*m*/*z*): 244 (M^+). Anal. Calcd for $C_{15}H_{16}OS$: C, 73.73; H, 6.60; S, 13.12. Found: C, 73.43; H, 6.46; S, 13.36.



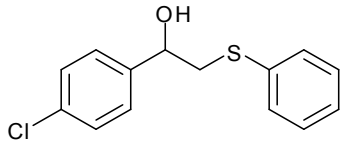
1-(4-methoxyphenyl)-2-(phenylthio)ethanol (4c)[10]

pale yellow oil; 88% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.22 (m, 7H), 6.90 (d, J = 8.5 Hz, 2H), 4.72 (dd, J = 9.3, 3.6 Hz, 1H), 3.83 (s, 3H), 3.34 (dd, J = 13.8, 3.6 Hz, 1H), 3.12 (dd, J = 13.8, 9.2 Hz, 1H), 2.83 (br s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.35, 135.07, 134.28, 130.13, 129.10, 127.16, 126.74, 113.98, 71.32, 55.33, 43.86. EIMS (*m*/*z*): 260 (M^+). Anal. Calcd for $C_{15}H_{16}O_2S$: C, 69.20; H, 6.19; S, 12.32. Found: C, 68.98; H, 6.12; S, 12.66.



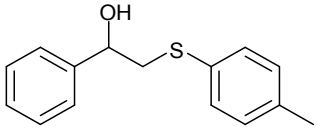
1-(4-bromophenyl)-2-(phenylthio)ethanol (4d)[9]

Pale yellow oil; 88% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.38 (m, 4H), 7.34-7.18 (m, 5H), 4.61 (d, J = 9.7 Hz, 1H), 3.27 (dd, J = 3.6, 13.4 Hz, 1H), 3.01-2.92 (m, 1H), 2.83 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.10, 134.81, 131.43, 130.26, 129.08, 126.82, 125.81, 122.44, 71.63, 44.14. EIMS (*m*/*z*): 307 (M^+). Anal. Calcd for $C_{14}H_{13}BrOS$: C, 54.38; H, 4.24; S, 10.37. Found: C, 54.59; H, 4.42; S, 10.09.



1-(4-chlorophenyl)-2-(phenylthio)ethanol (4e)[11]

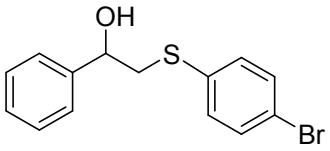
Oil; 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.41(m, 2 H), 7.36-7.27 (m, 7 H), 4.72 (dd, J = 9.4, 3.6 Hz, 1H), 3.29 (dd, J = 13.7, 3.6 Hz, 1 H), 3.08-3.00 (m, 2 H, including br s, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.66, 134.52, 133.64, 130.42, 129.27, 128.62, 127.25, 126.91, 71.08, 44.02. EIMS (*m*/*z*): 264 (M^+). Anal. Calcd for $C_{14}H_{13}ClOS$: C, 63.51; H, 4.95; S, 13.39. Found: C, 63.25; H, 5.13; S, 13.56.



1-phenyl-2-(p-tolylthio)ethanol (4f)[12]

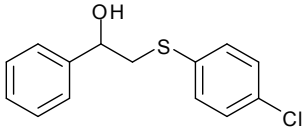
Oil; 95% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.21 (m, 7 H), 7.14 (d, J = 8.4 Hz, 2 H), 4.68 (dd, J = 9.8, 1.5 Hz, 1 H), 3.24 (dd, J = 13.6, 3.6 Hz, 1 H), 3.07-2.97 (m, 2 H, including br s, OH), 2.33 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.22, 137.12, 131.05, 130.96, 130.02,

128.53, 127.93, 125.82, 71.51, 44.86, 21.02. EIMS (*m*/*z*): 244 (M^+). Anal. Calcd for $C_{15}H_{16}OS$: C, 73.73; H, 6.60; S, 13.12. Found: C, 73.80; H, 6.36; S, 13.46.



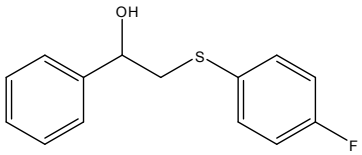
2-(4-bromophenylthio)-1-phenylethanol (4g)[9]

Pale yellow oil; 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 9.1 Hz, 2H), 7.36-7.27 (m, 7H), 4.76-4.70(m, 1H), 3.26 (dd, J = 3.6, 13.8 Hz, 1H), 3.14-3.05 (m, 1H), 2.62 (d, 1H, J = 2.2 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.22, 133.90, 132.03, 129.94, 128.51, 128.11, 126.63, 120.23, 71.60, 43.81. EIMS (*m*/*z*): 307 (M^+). Anal. Calcd for $C_{14}H_{13}BrOS$: C, 54.38; H, 4.24; S, 10.37. Found: C, 54.08; H, 4.40; S, 10.17.



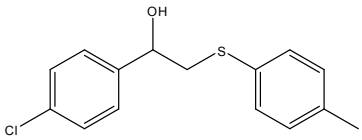
2-(4-chlorophenylthio)-1-phenylethanol (4h)[11]

Oil; 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.27 (m, 9 H), 4.73 (dd, J = 9.1, 4.2 Hz, 1 H), 3.25 (dd, J = 13.7, 4.2 Hz, 1 H), 3.15-3.07 (m, 1 H), 2.84 (br s, 1 H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.89, 131.21, 129.54, 129.03, 128.44, 127.92, 125.63, 125.20, 71.64, 43.82. EIMS (*m*/*z*): 264 (M^+). Anal. Calcd for $C_{14}H_{13}ClOS$: C, 63.51; H, 4.95; S, 12.11. Found: C, 63.60; H, 4.76; S, 11.99.



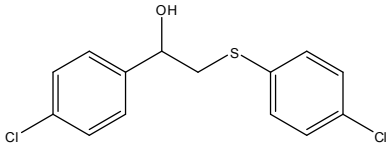
2-(4-fluorophenylthio)-1-phenylethanol (4i)

Oil; 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44-7.30 (m, 7 H), 7.05-6.97 (m, 2 H), 4.70 (dd, J = 9.3, 3.7 Hz, 1 H), 3.26 (dd, J = 13.6, 3.7 Hz, 1 H), 3.12-3.03 (m, 1 H), 2.88 (br s, 1 H, OH); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.11(d, JC-F = 245.8 Hz, 1 C), 142.04, 133.12 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.89 (d, $J_{C\text{-}F}$ = 3.3 Hz), 128.54, 128.06, 125.83, 116.22 (d, $J_{C\text{-}F}$ = 21.8 Hz), 71.76, 45.14; EIMS (*m*/*z*): 248 (M^+). Anal. Calcd for $C_{14}H_{13}FOS$: C, 67.72; H, 5.28; S, 12.91; Found: C, 67.42; H, 5.22, S, 13.13.



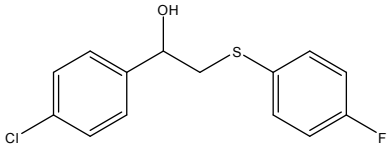
1-(4-chlorophenyl)-2-(p-tolylthio)ethanol (4j)

Oil; 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33-7.20 (m, 6 H), 7.13 (d, *J* = 8.0 Hz, 2 H), 4.67-4.60 (m, 1 H), 3.18 (dd, *J* = 13.8, 3.5 Hz, 1 H), 2.99-2.92 (m, 2 H), 2.36 (s, 3 H), ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.64, 137.38, 133.52, 131.22, 130.51, 130.04, 128.69, 127.25, 70.72, 44.98, 21.07; EIMS (*m*/*z*): 278 (M^+). Anal. Calcd for $C_{15}H_{15}ClOS$: C, 64.62; H, 5.42; S, 11.50. Found: C, 64.32; H, 5.59; S, 11.65.



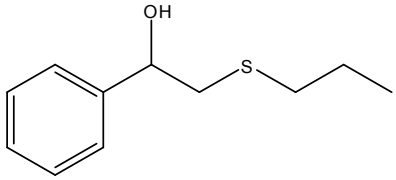
1-(4-chlorophenyl)-2-(4-chlorophenylthio)ethanol (4k)

Oil; 81% yield; 1H NMR (400 MHz, $CDCl_3$) δ: 7.35-7.21 (m, 8 H), 4.64 (dd, *J* = 9.0, 3.9, 1 H), 3.23 (dd, *J* = 13.8, 3.9 Hz, 1 H), 3.09-3.02 (m, 1 H) 2.95 (br s, 1 H, OH); ^{13}CNMR (100 MHz, $CDCl_3$) δ: 140.33, 133.54, 133.10, 132.87, 131.42, 129.63, 129.14, 128.57, 127.06, 126.86, 125.12, 70.94, 43.80; EIMS (*m*/*z*): 298 (M^+). Anal. Calcd for $C_{14}H_{12}Cl_2OS$: C, 56.20; H, 4.04; S, 10.72. Found: C, 56.25; H, 4.16; S, 10.46.



1-(4-chlorophenyl)-2-(4-fluorophenylthio)ethanol (4l)

Oil; 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45-7.36 (m, 2 H), 7.33-7.22 (m, 4 H), 7.06 (t, *J* = 6.8 Hz, 2H), 4.63 (dd, *J* = 9.1, 3.9, 1 H), 3.19 (dd, *J* = 3.9, 13.8 Hz, 1 H), 3.06-2.98 (m, 2 H, including br s, OH); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.20 (d, $J_{C\text{-}F}$ = 246.3 Hz), 140.46, 133.65, 133.37 (d, *J*C-F = 8.1 Hz), 129.51 (d, $J_{C\text{-}F}$ = 3.3 Hz), 128.64, 127.22, 116.35(d, $J_{C\text{-}F}$ = 21.7 Hz), 71.00, 45.04; EIMS (*m*/*z*): 282 (M^+). Anal. Calcd for $C_{14}H_{12}ClFOS$: C, 59.47; H, 4.28; S, 11.34. Found: C, 59.34; H, 4.49; S, 11.01.



1-phenyl-2-(propylthio)ethanol (4m)

Oil; 87% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.26 (m, 5 H), 4.37 (dd, *J* = 9.4, 3.4, 1 H), 3.02-2.99 (br s, 1 H, OH), 2.93 (dd, *J* = 13.7, 3.5 Hz, 1 H), 2.71 (dd, *J* = 13.7, 9.4 Hz, 1 H), 2.52 (t, *J* = 6.9 Hz, 2 H), 1.66-1.60 (m, 2 H), 0.99 (t, *J* = 7.3 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:142.53, 128.53, 127.85, 125.80, 71.57, 42.11, 34.16, 23.00, 13.43; EIMS (*m*/*z*): 196 (M^+). Anal. Calcd for $C_{11}H_{16}OS$: C, 67.30; H, 8.22; S, 16.33. Found: C, 67.61; H, 7.94; S, 16.41.

iv. References

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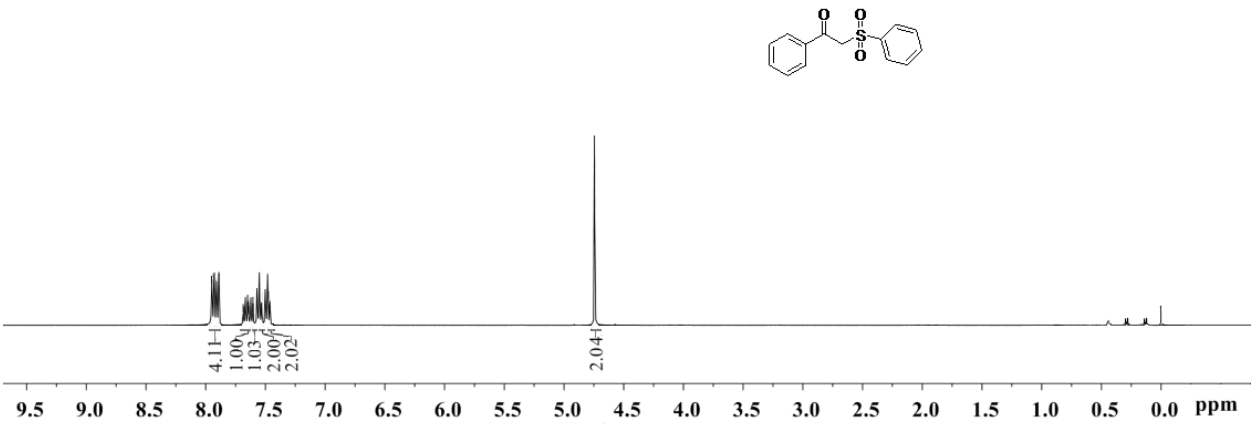
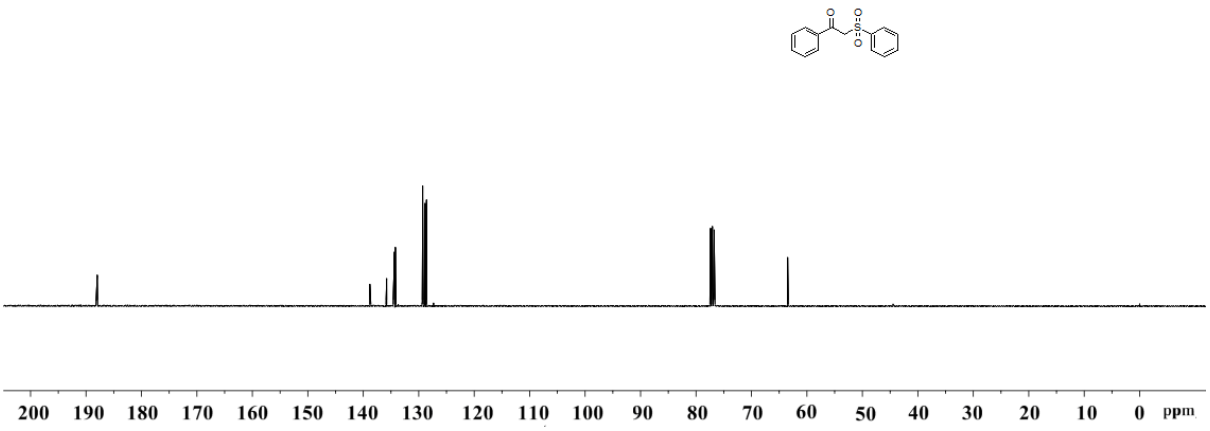
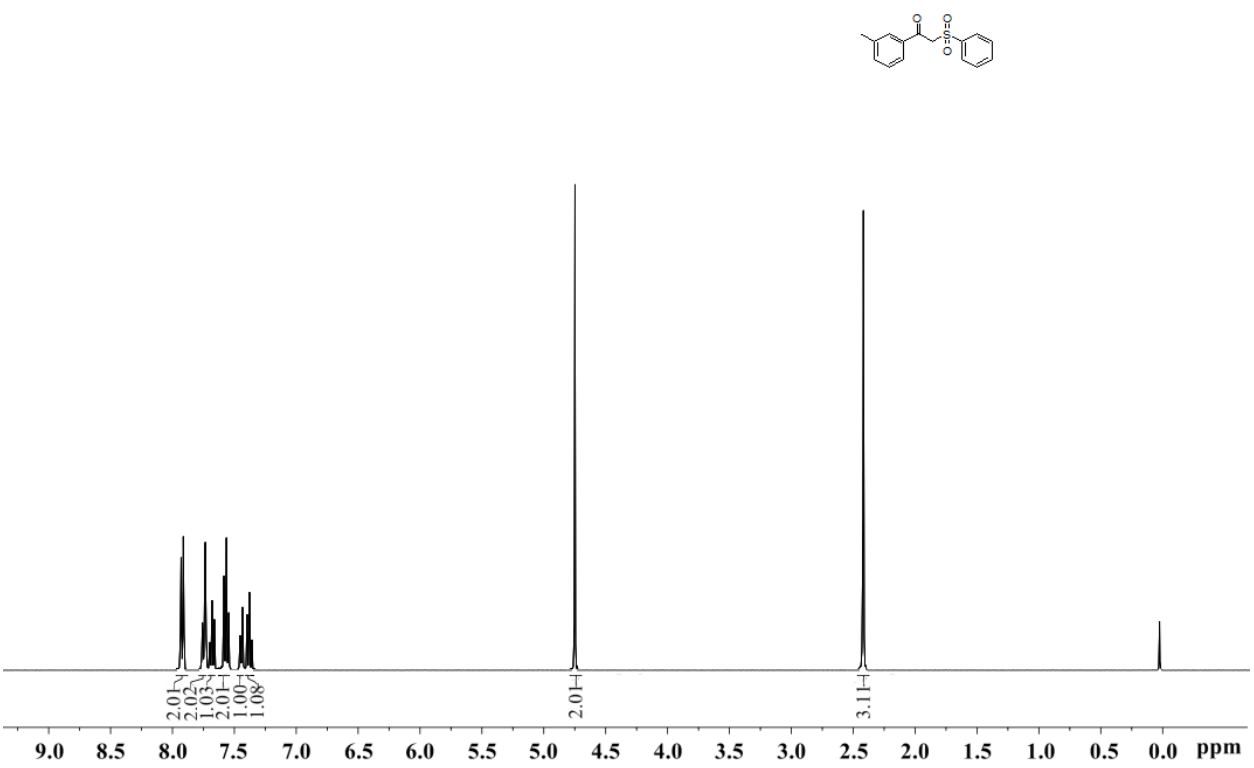
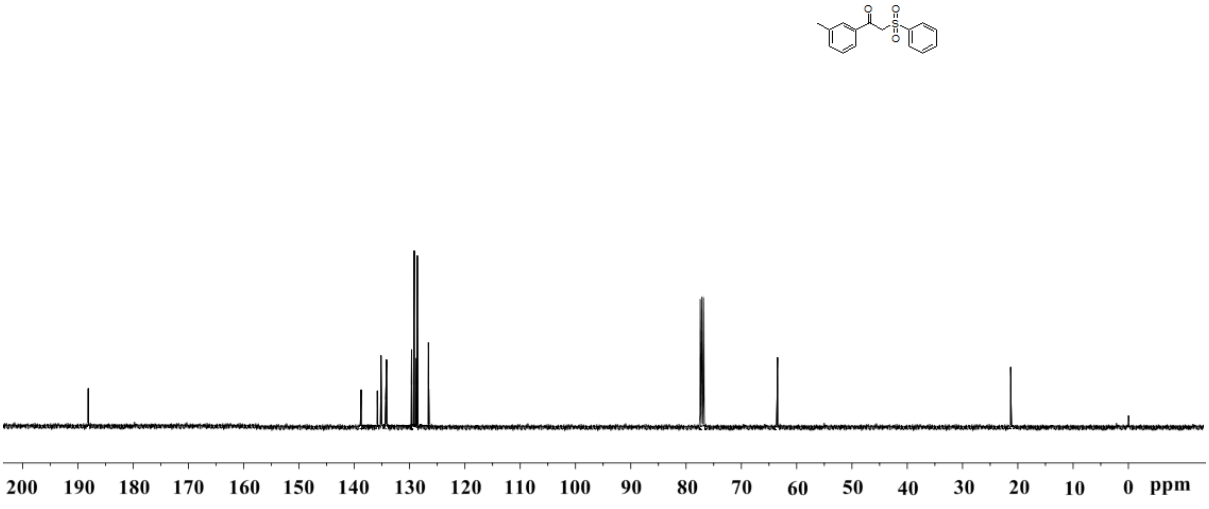
v. NMR spectra of products **3** and **4**






2.01
2.02
1.03
2.01
1.00
1.08
2.01
3.11
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 0.0 ppm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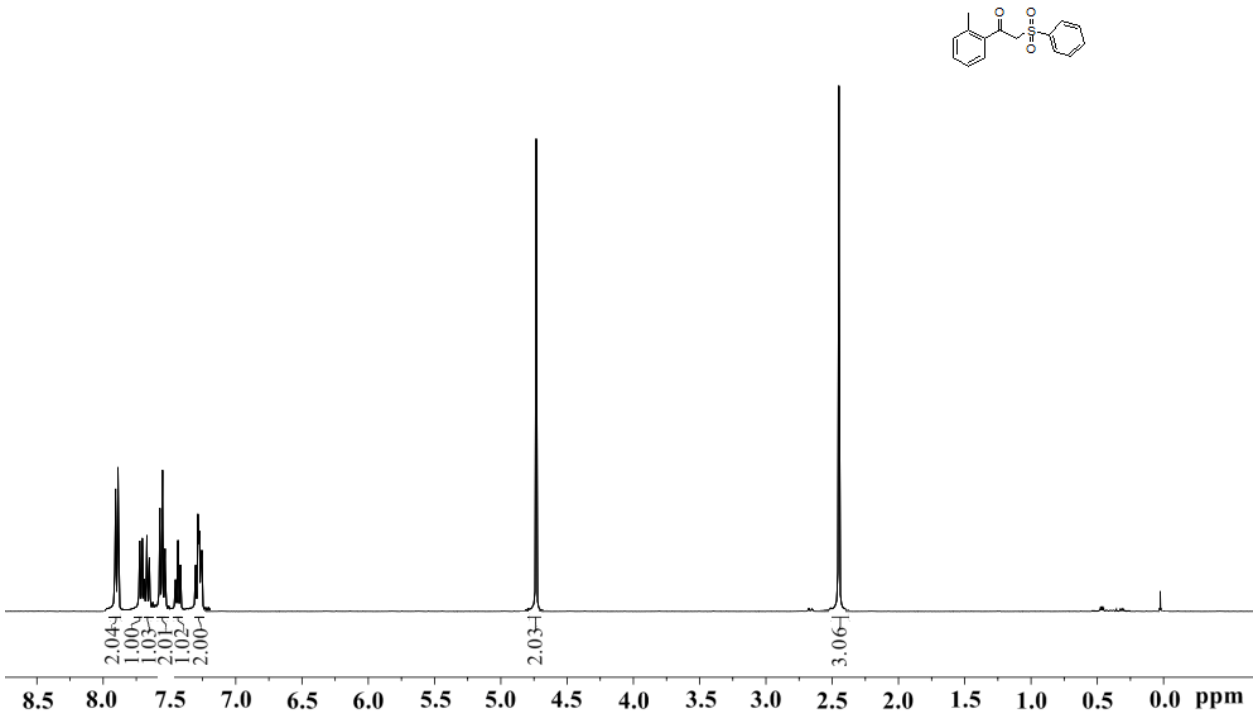
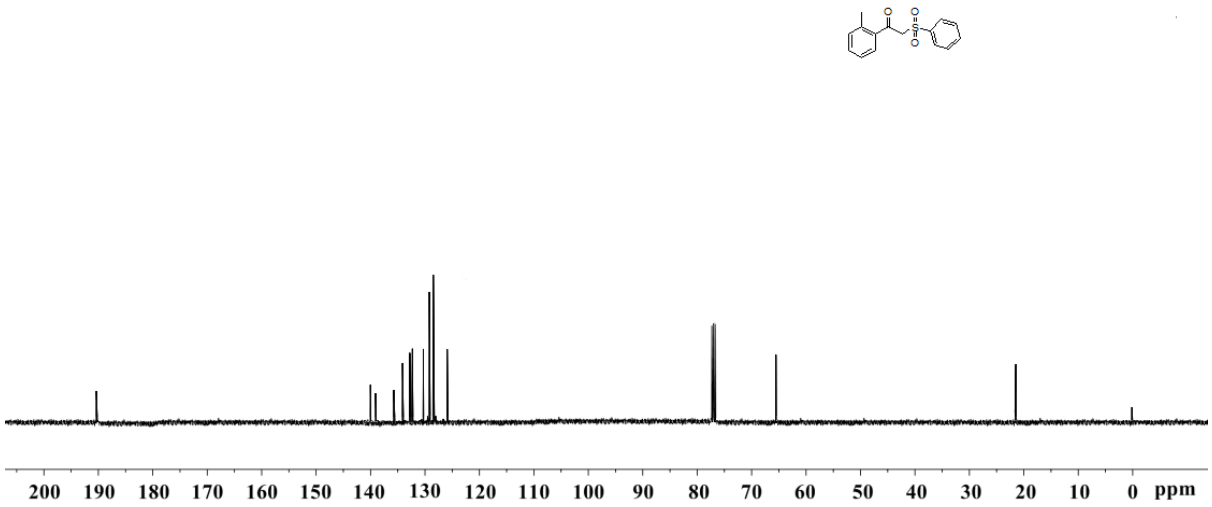

2.04
1.00
1.03
2.01
1.02
2.00
2.03
3.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm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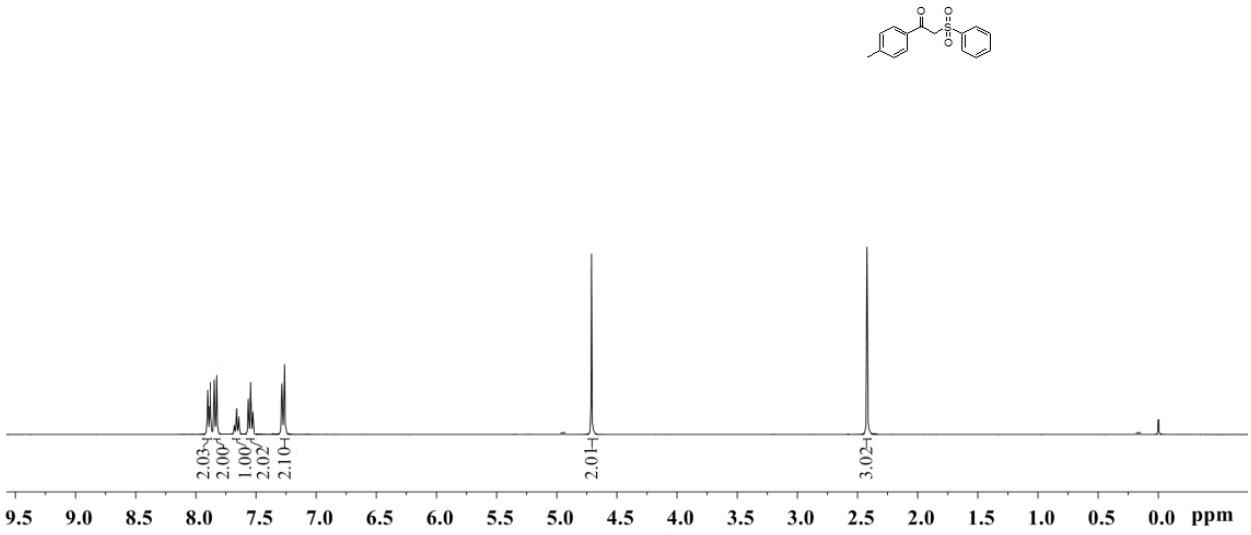
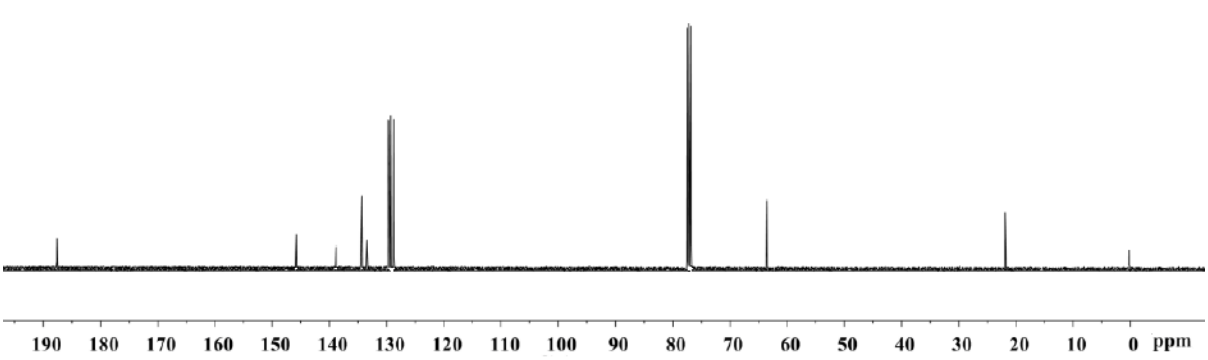

2.03
2.00
1.00
2.02
2.10
2.01
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm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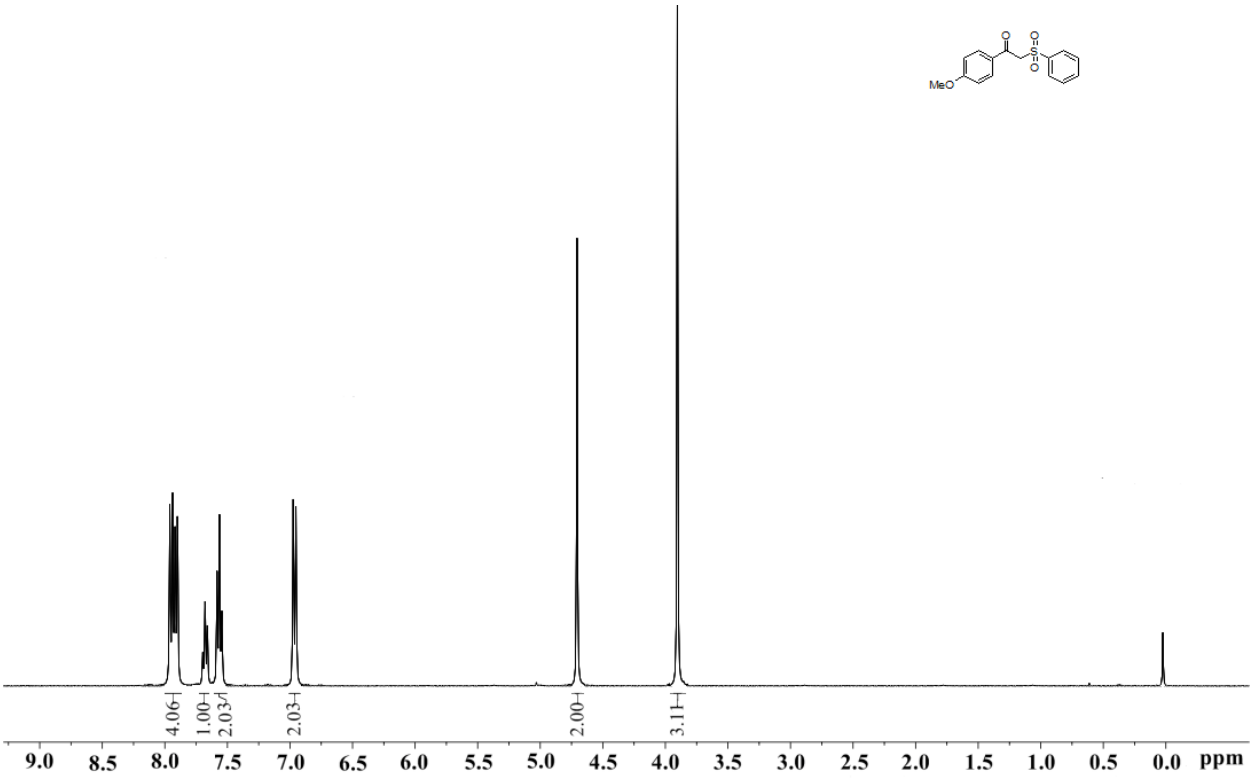
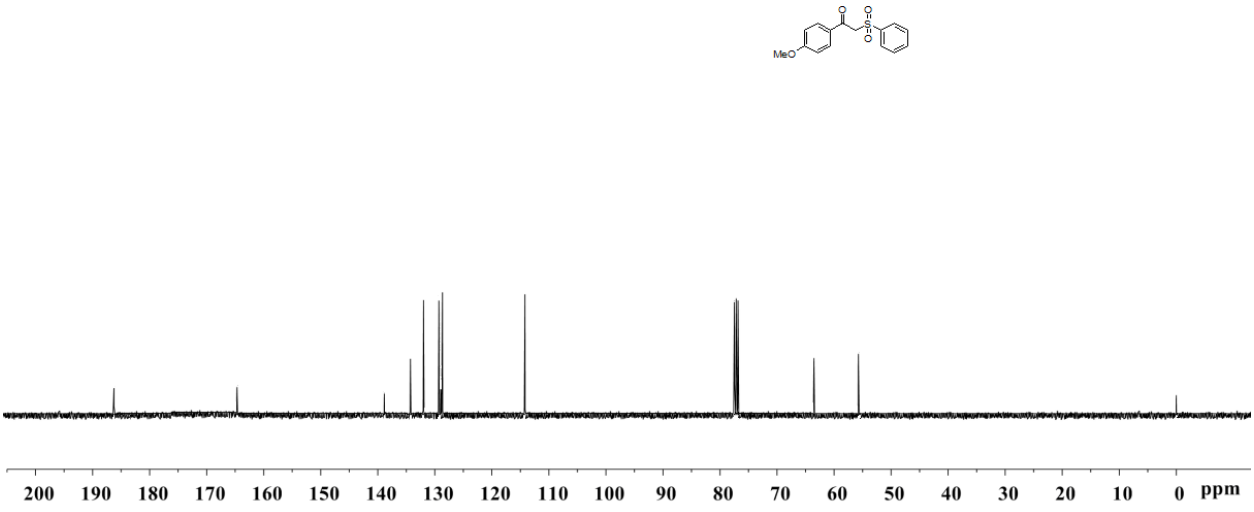
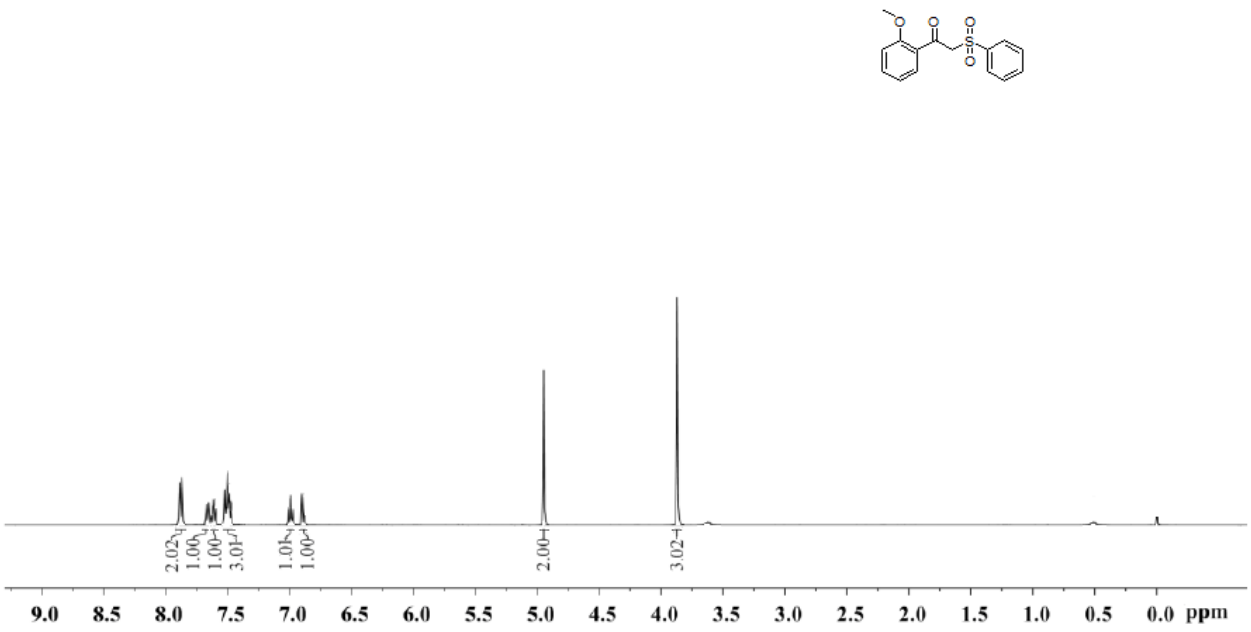
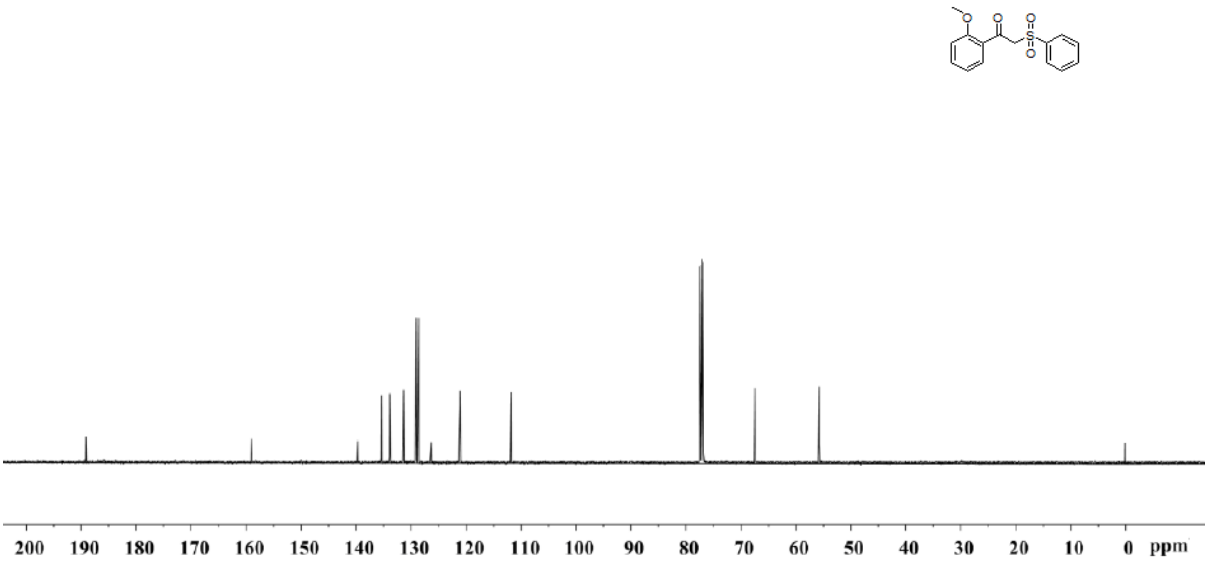

MeO
4.06
1.00
2.03
2.03
2.00
3.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


MeO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


2.02
1.00
1.00
3.01
1.01
1.00
2.00
3.02
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 0.0 ppm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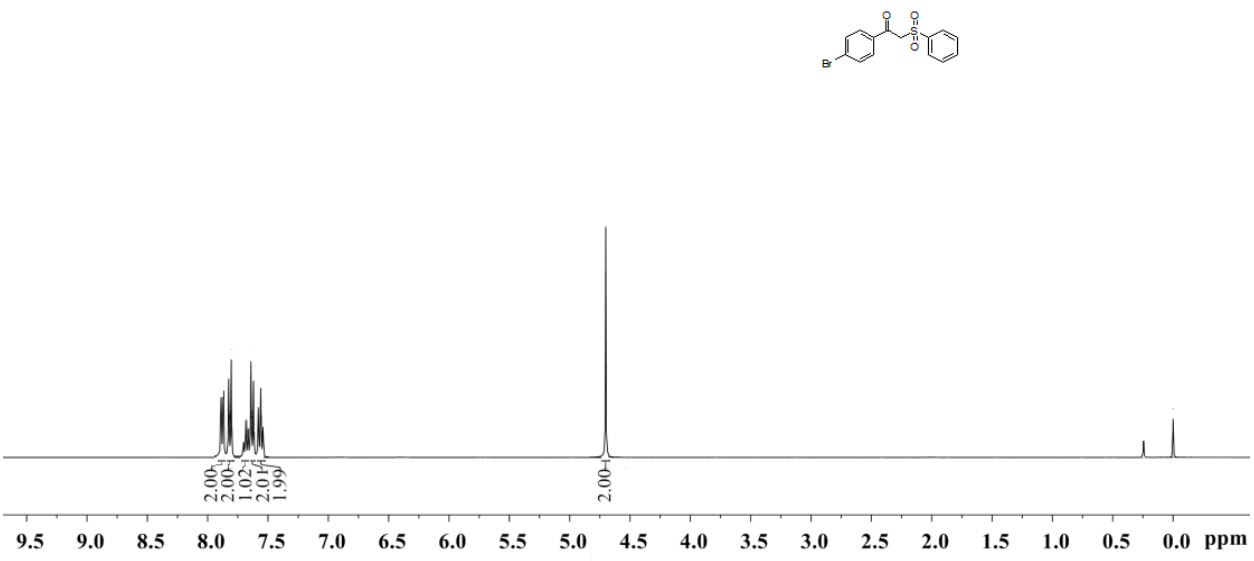
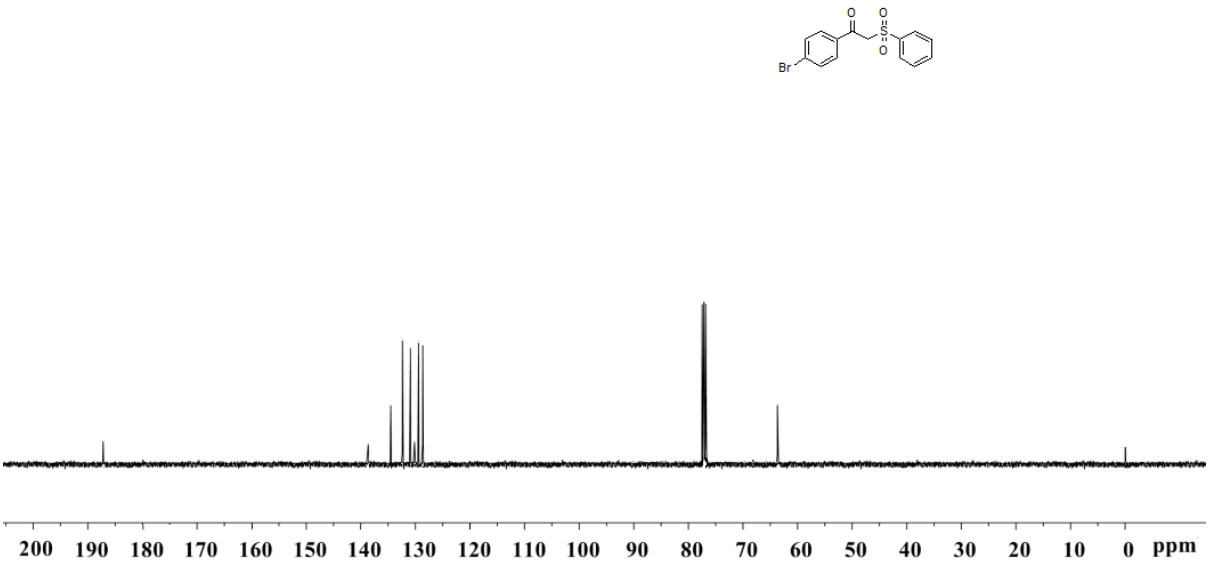

2.00
2.00
1.02
2.01
1.99
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm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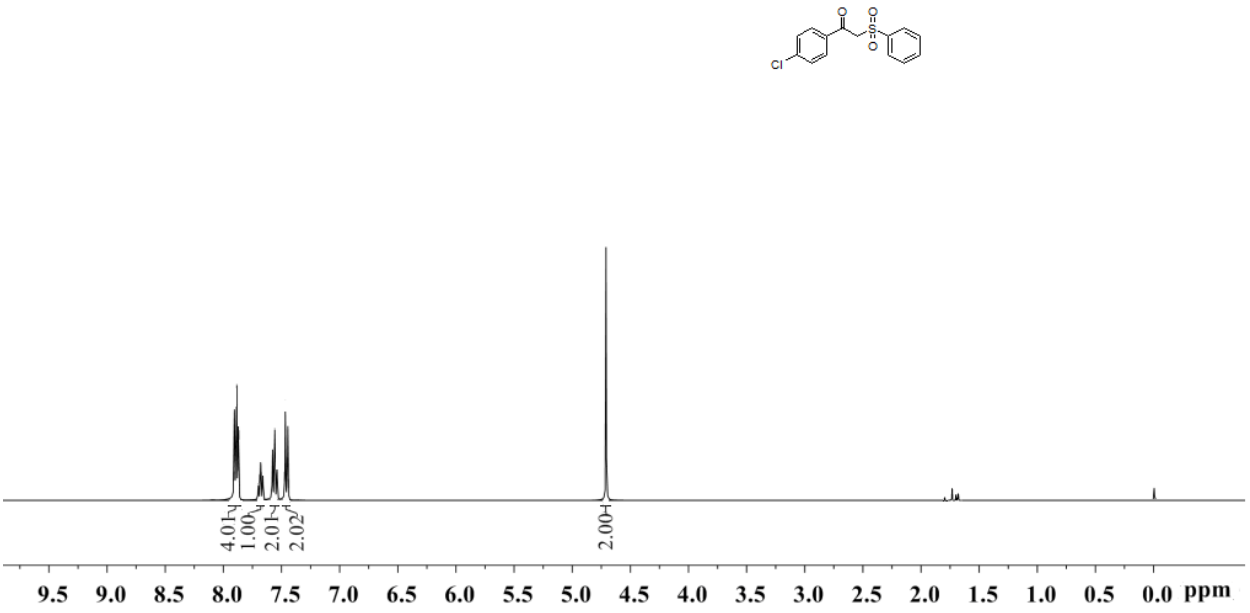
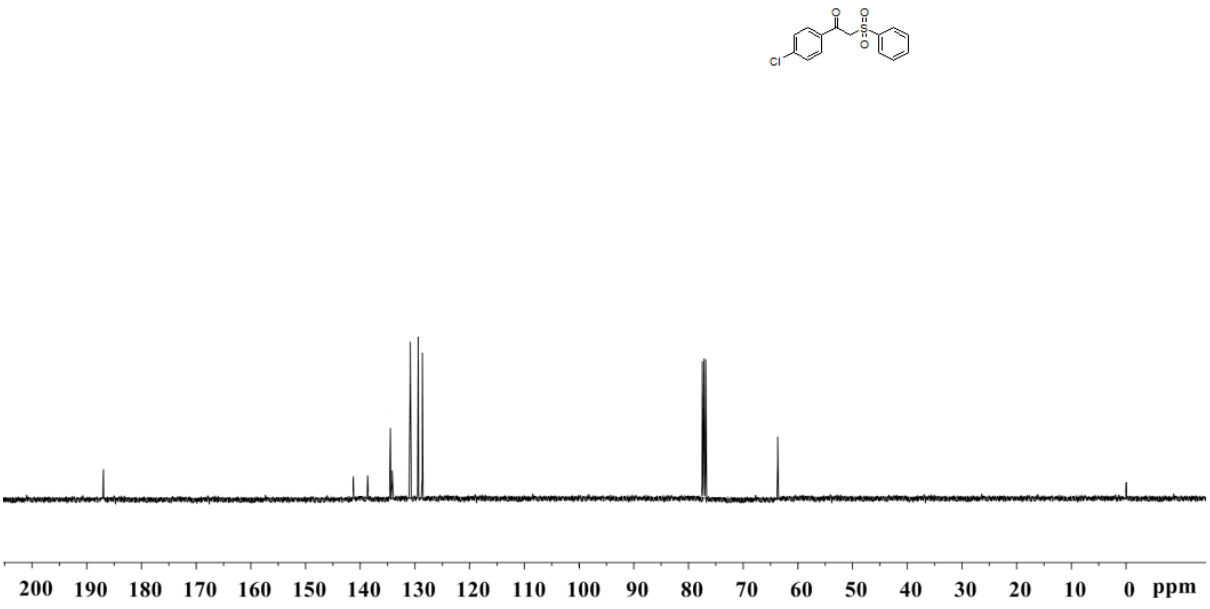

4.01H
1.00H
2.01H
2.02H
2.00H
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm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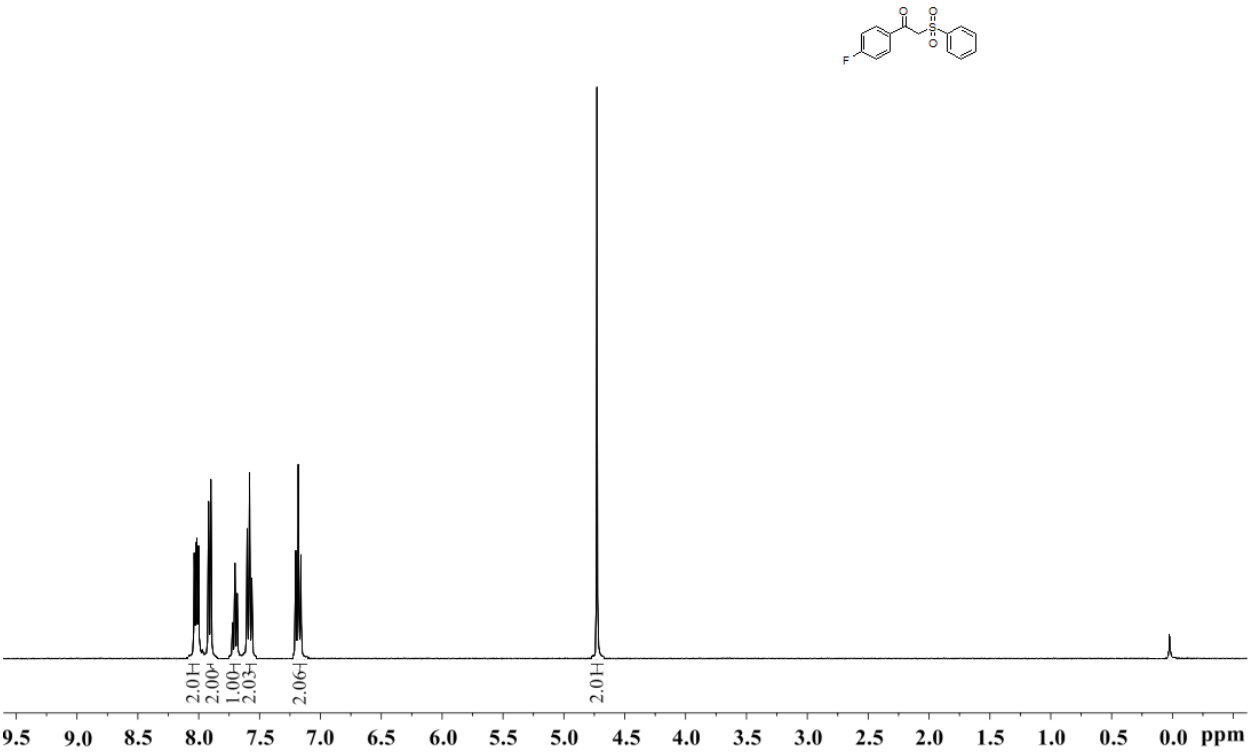
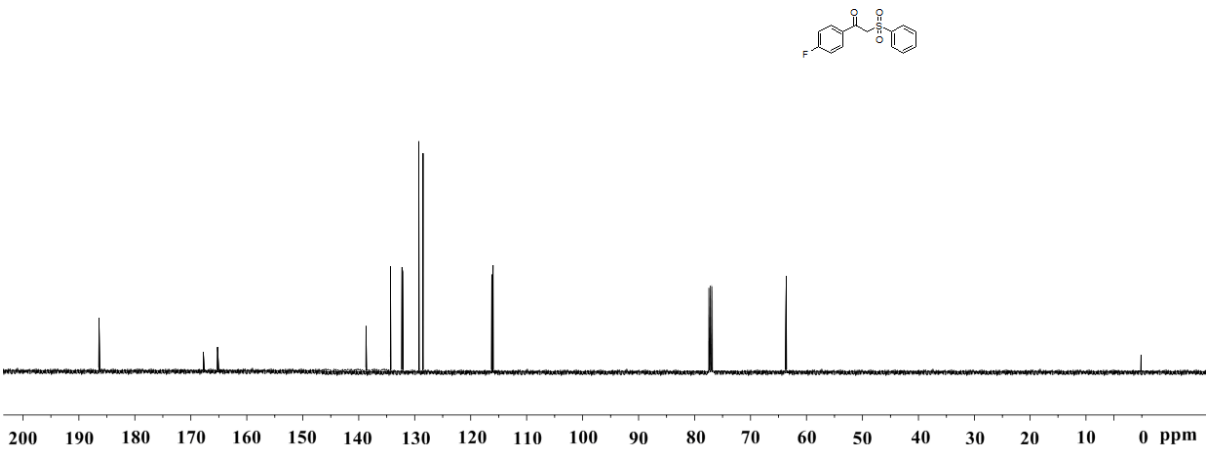
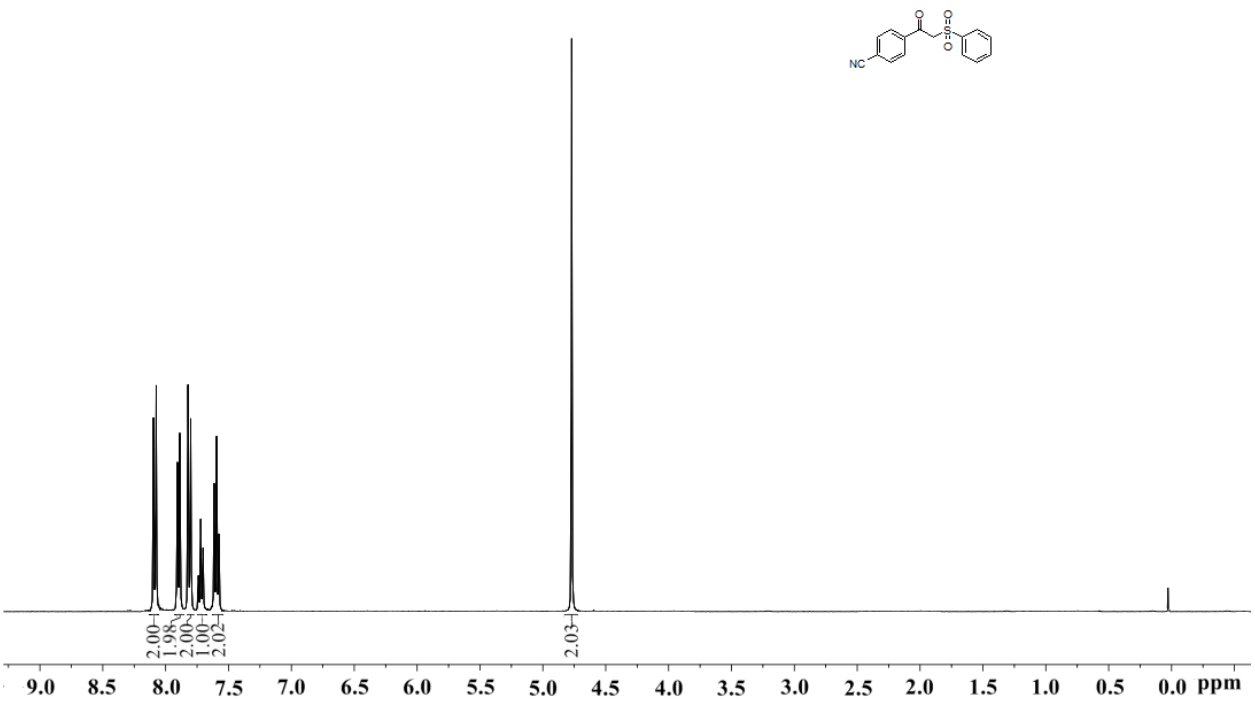
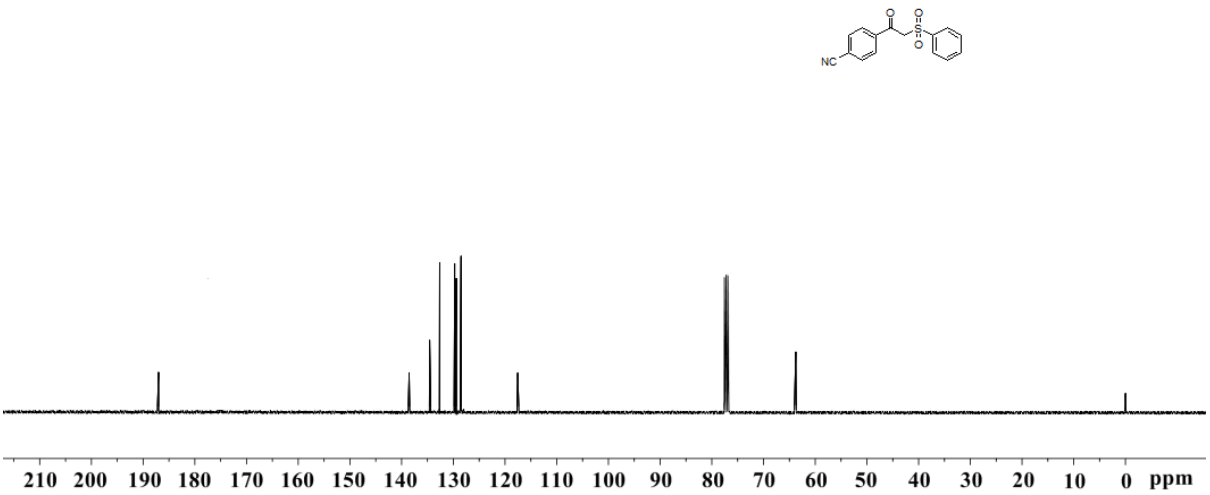
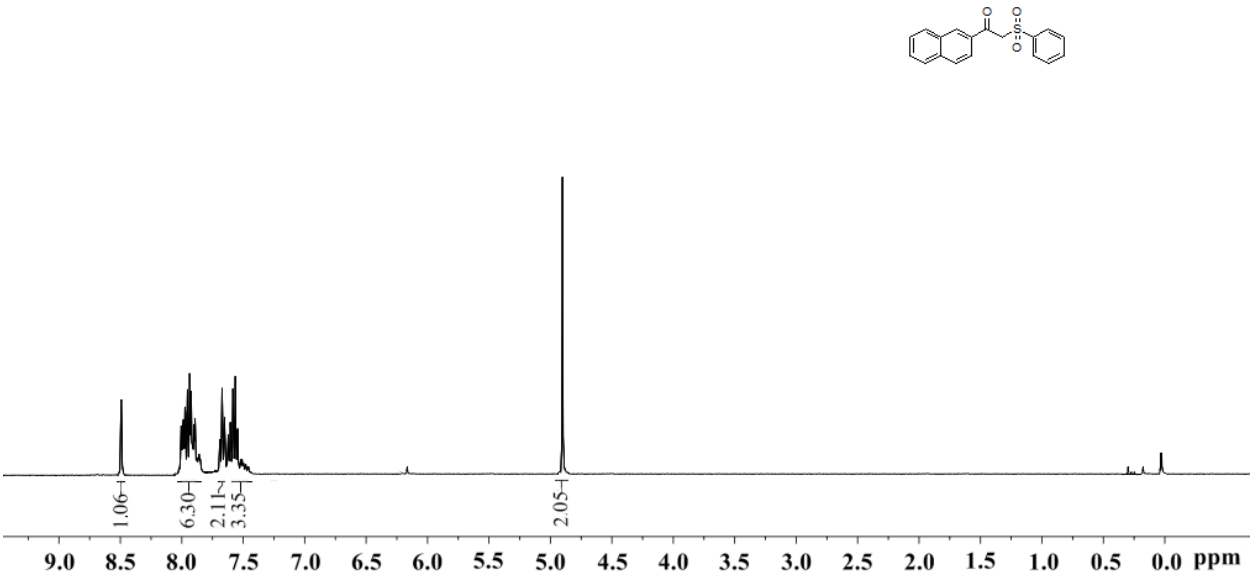
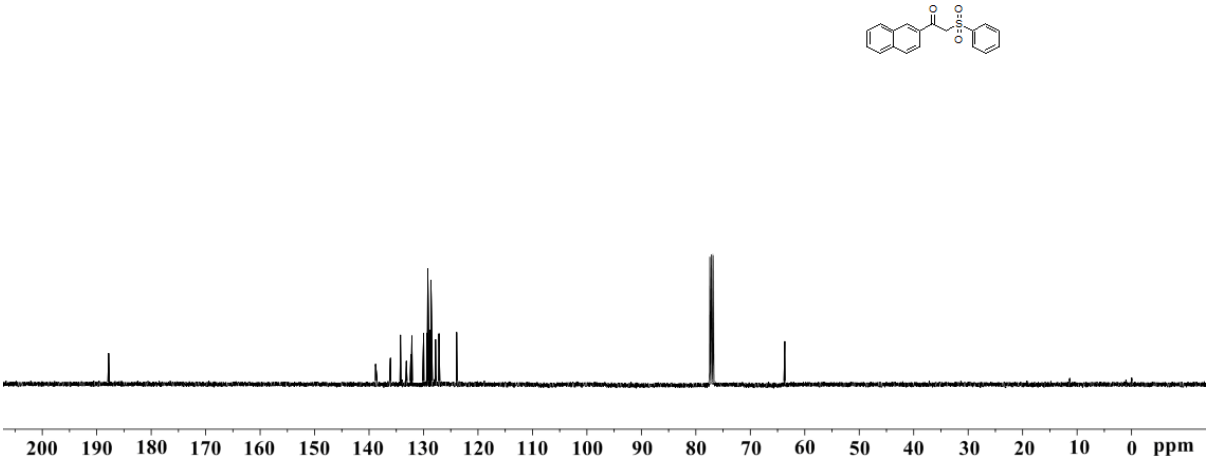

2.01H
2.00H
1.00H
2.03H
2.06H
2.01H
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

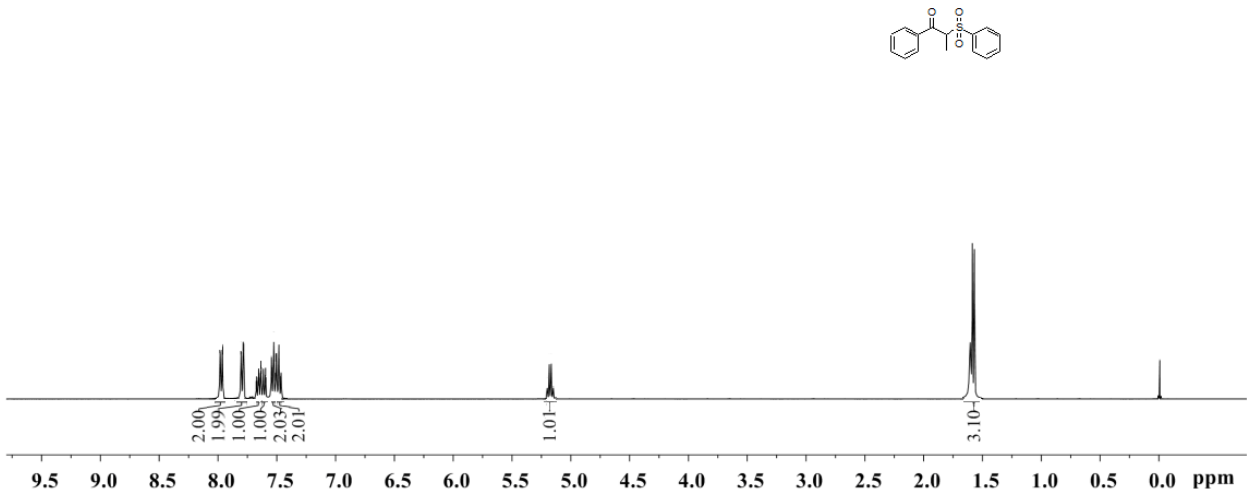

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

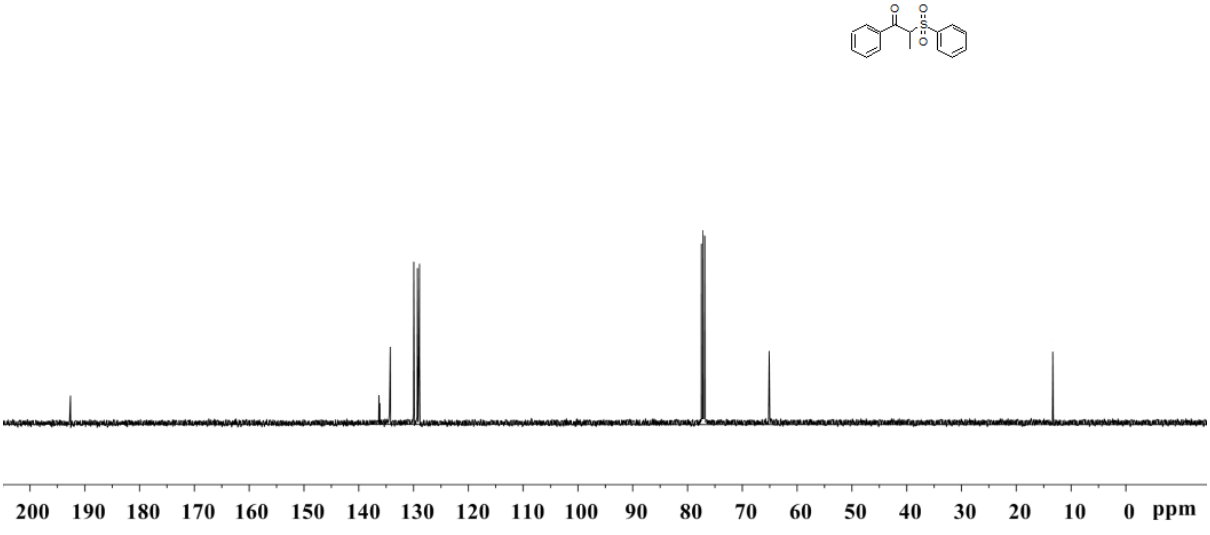

NC
2.00
1.98
2.00
1.00
2.02
2.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


1.06
6.30
2.11
3.35
2.05
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 0.0 ppm


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


2.00
1.99
1.00
1.00
2.03
2.01
1.01
3.10
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 0.0 ppm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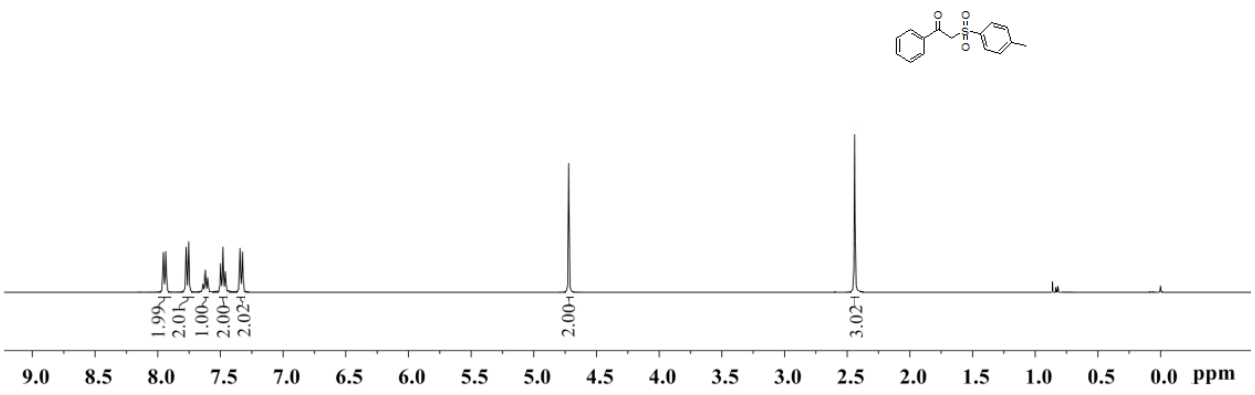
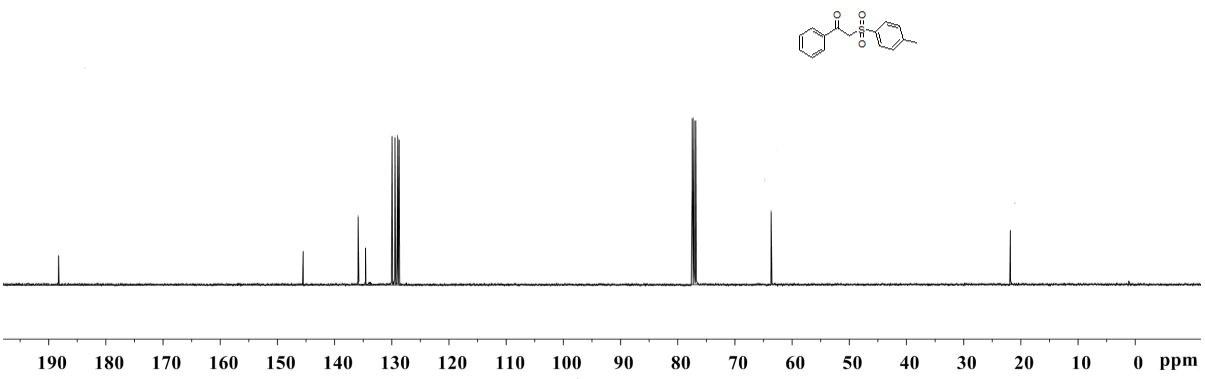
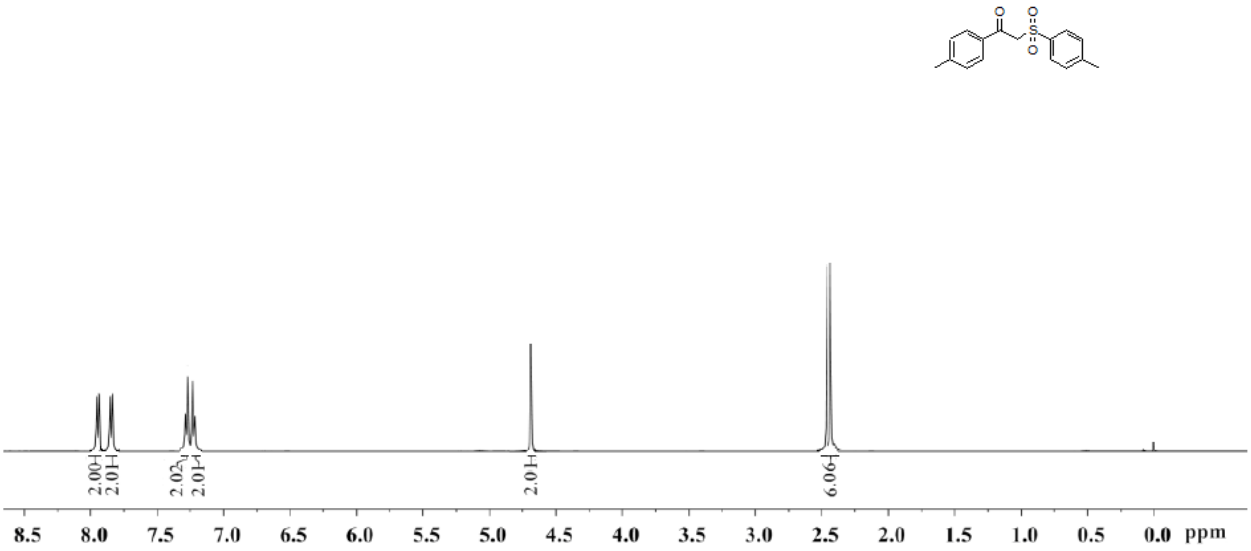
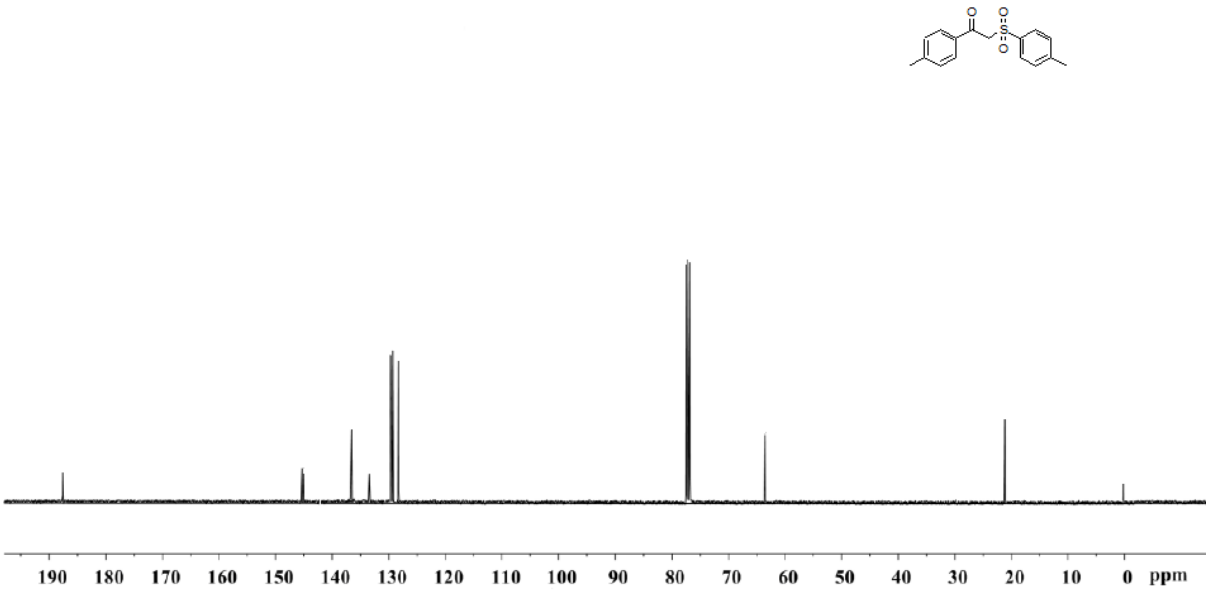
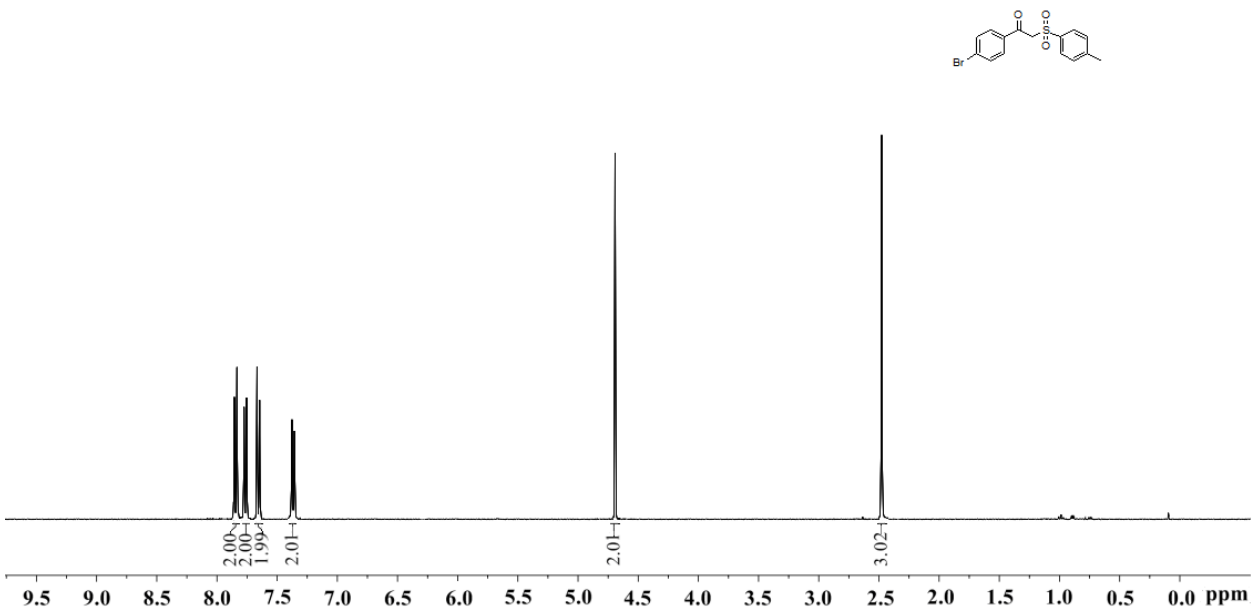
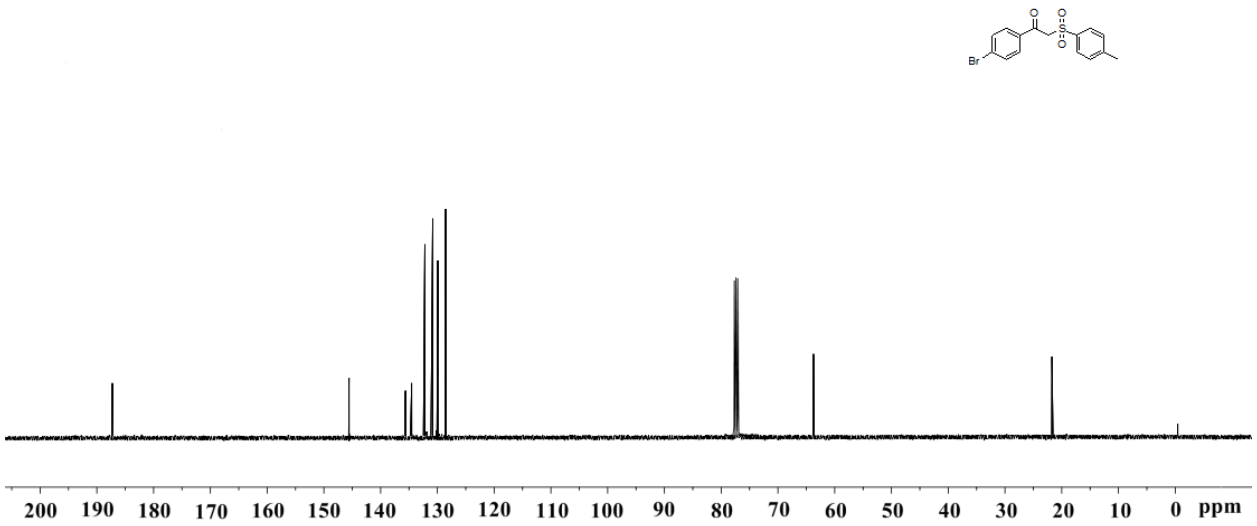

1.99
2.01
1.00
2.00
2.02
2.00
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

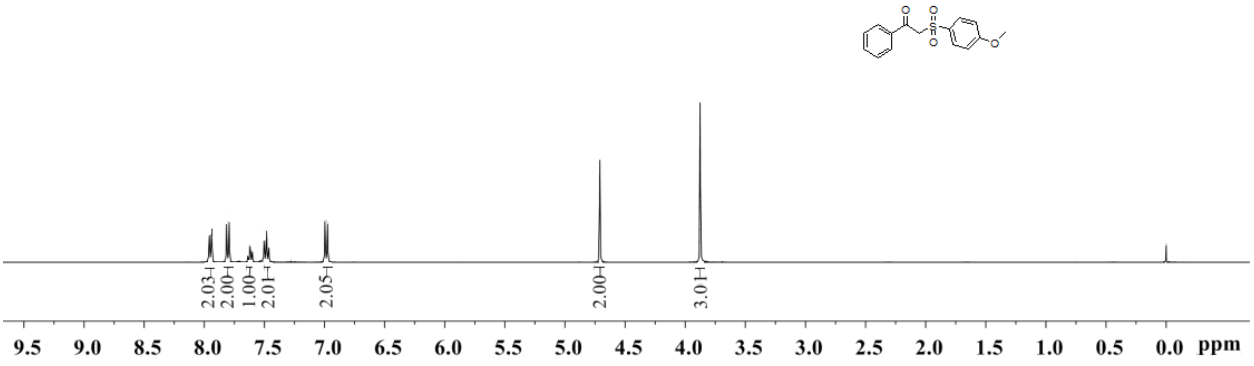

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

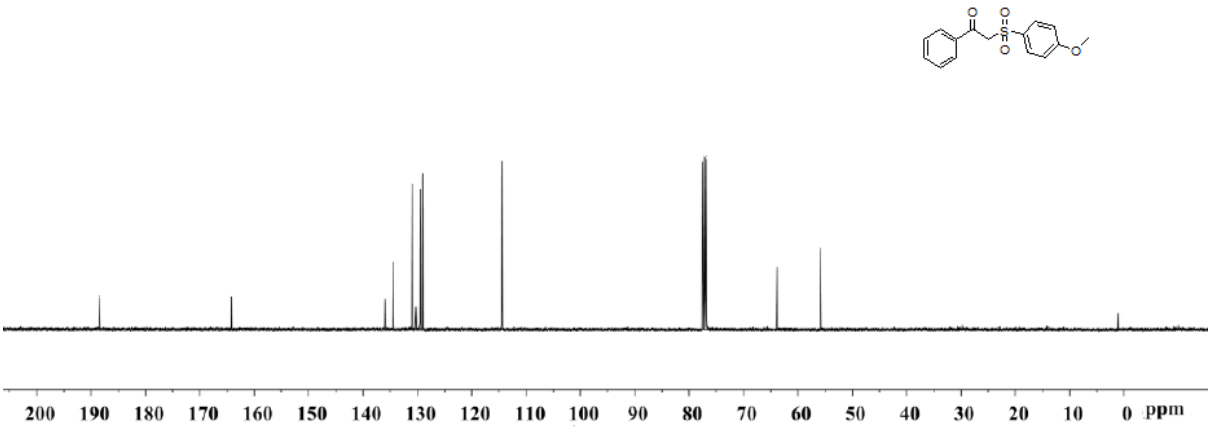

2.00
2.01
2.02
2.01
2.01
6.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

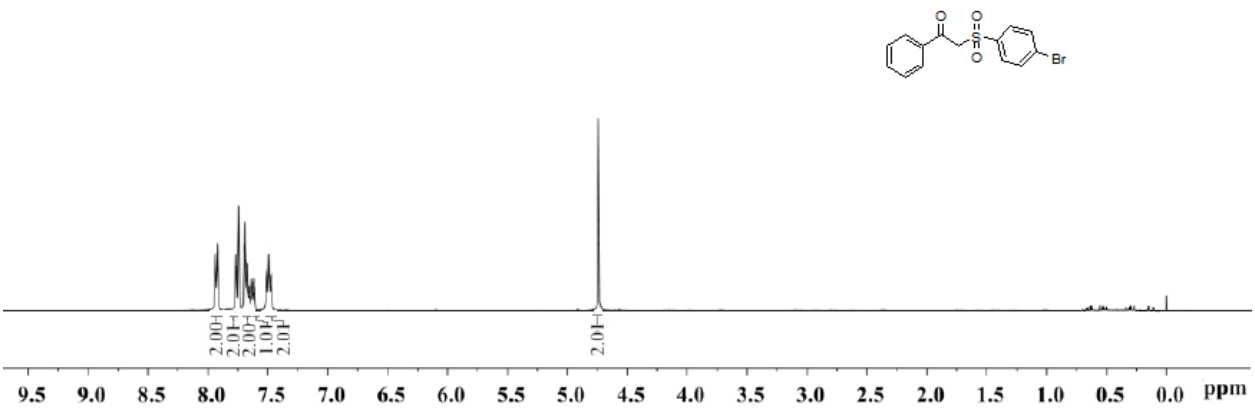

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

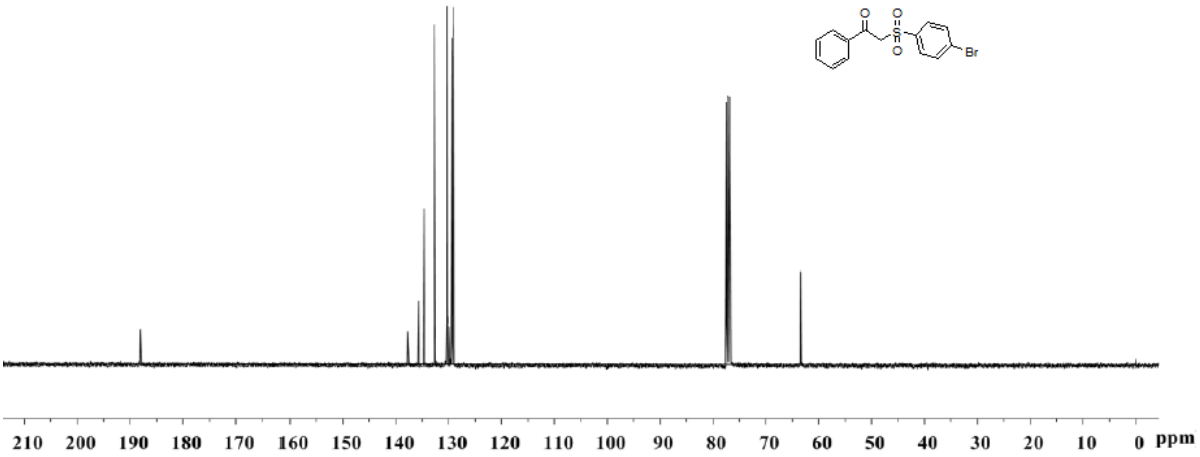

2.00
2.00
1.99
2.01
2.01
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

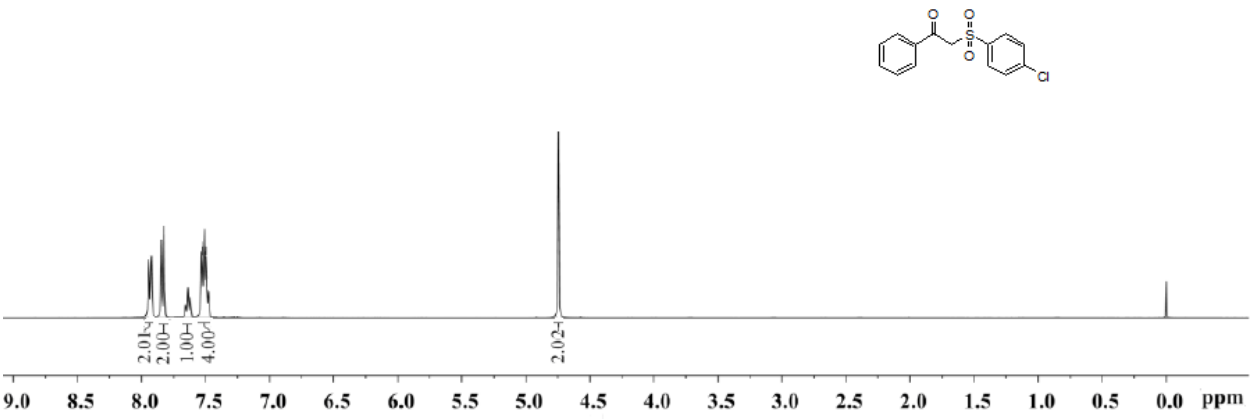

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

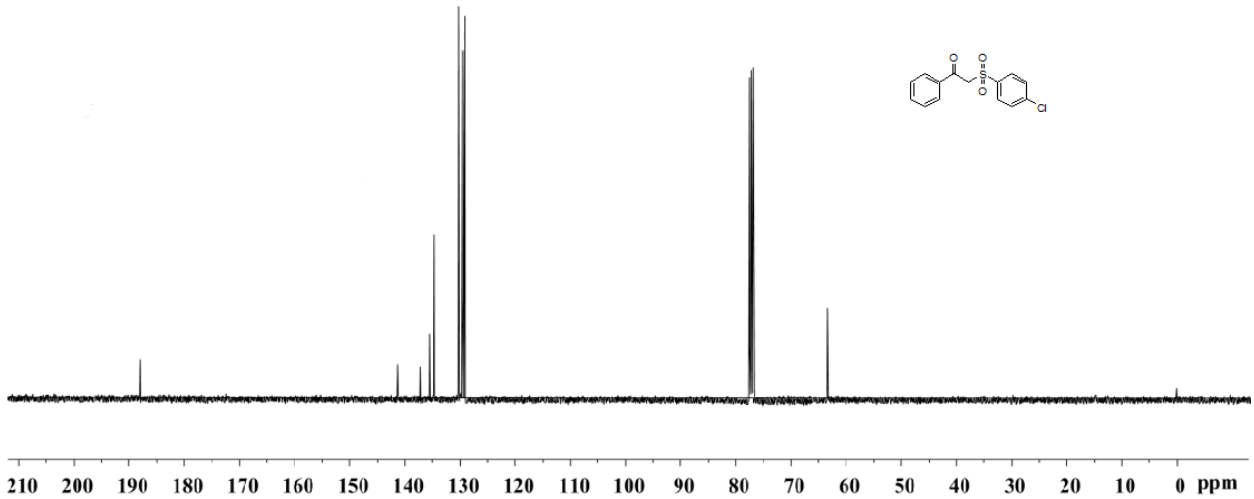

2.03
2.00
1.00
2.01
2.05
2.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

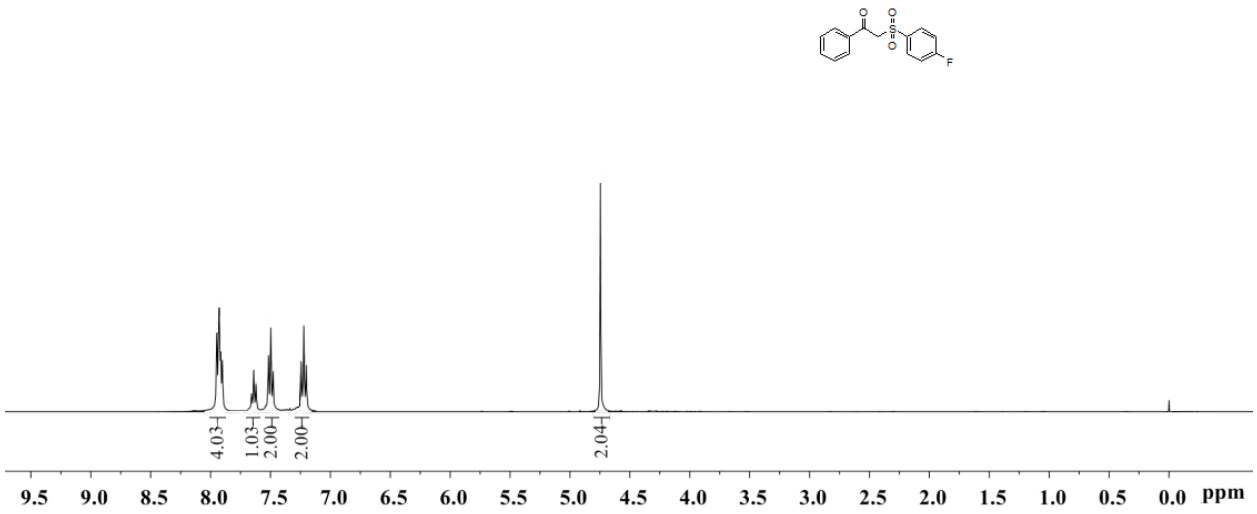

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

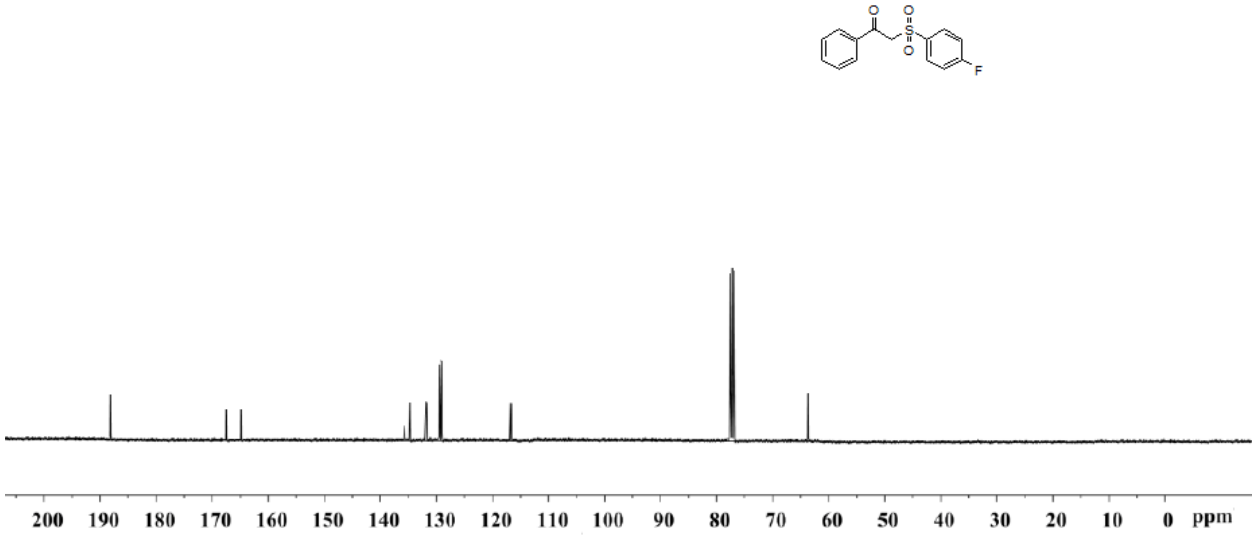

Br
2.00
2.01
2.00
1.01
2.01
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

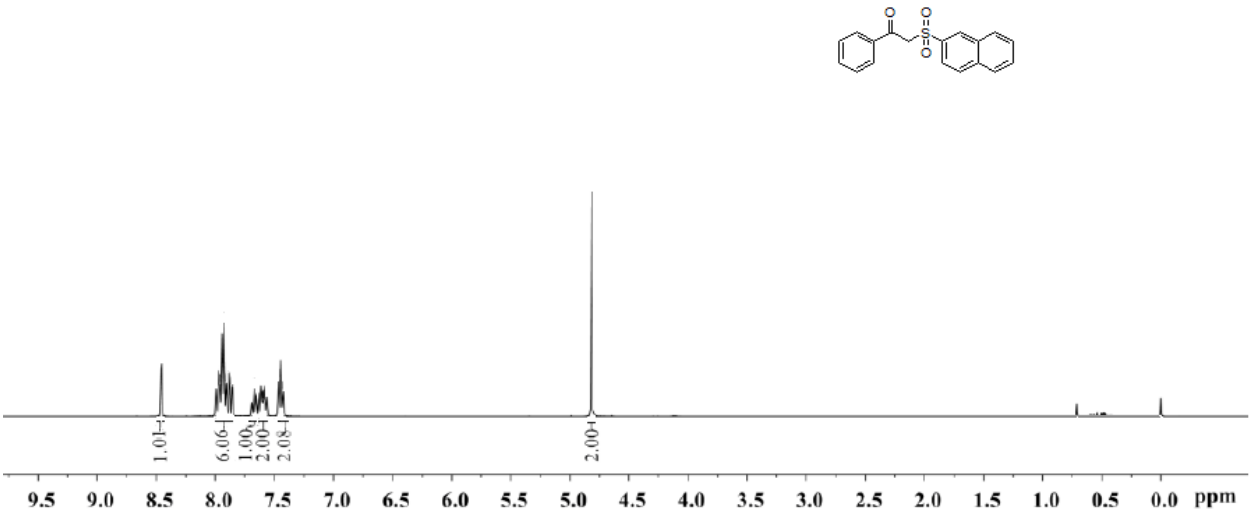

Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

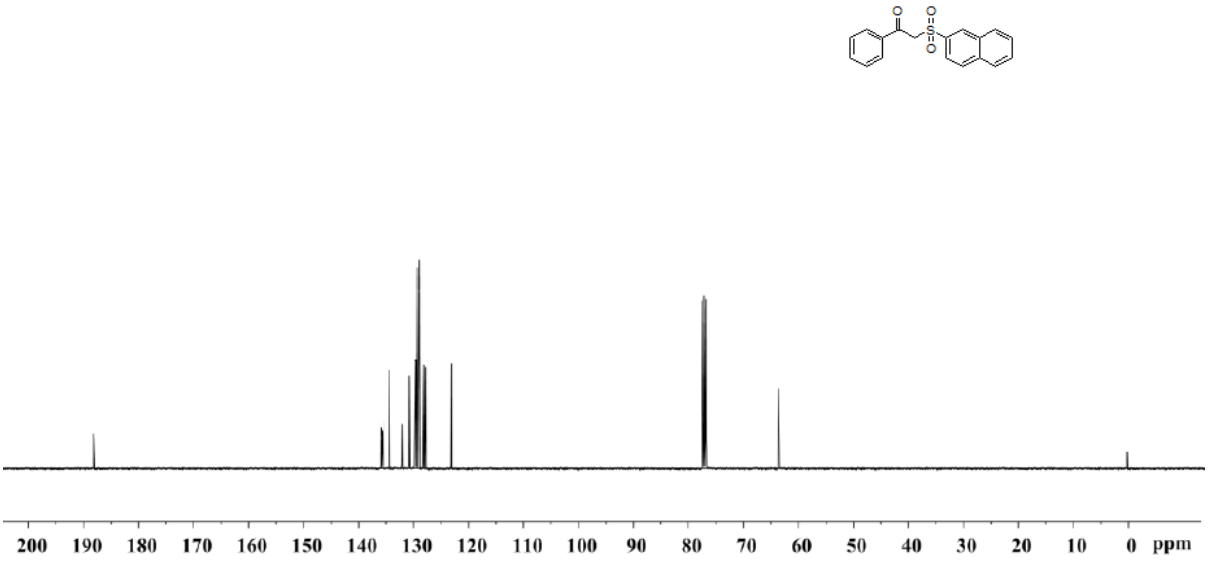

2.01
2.00
1.00
4.00
2.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

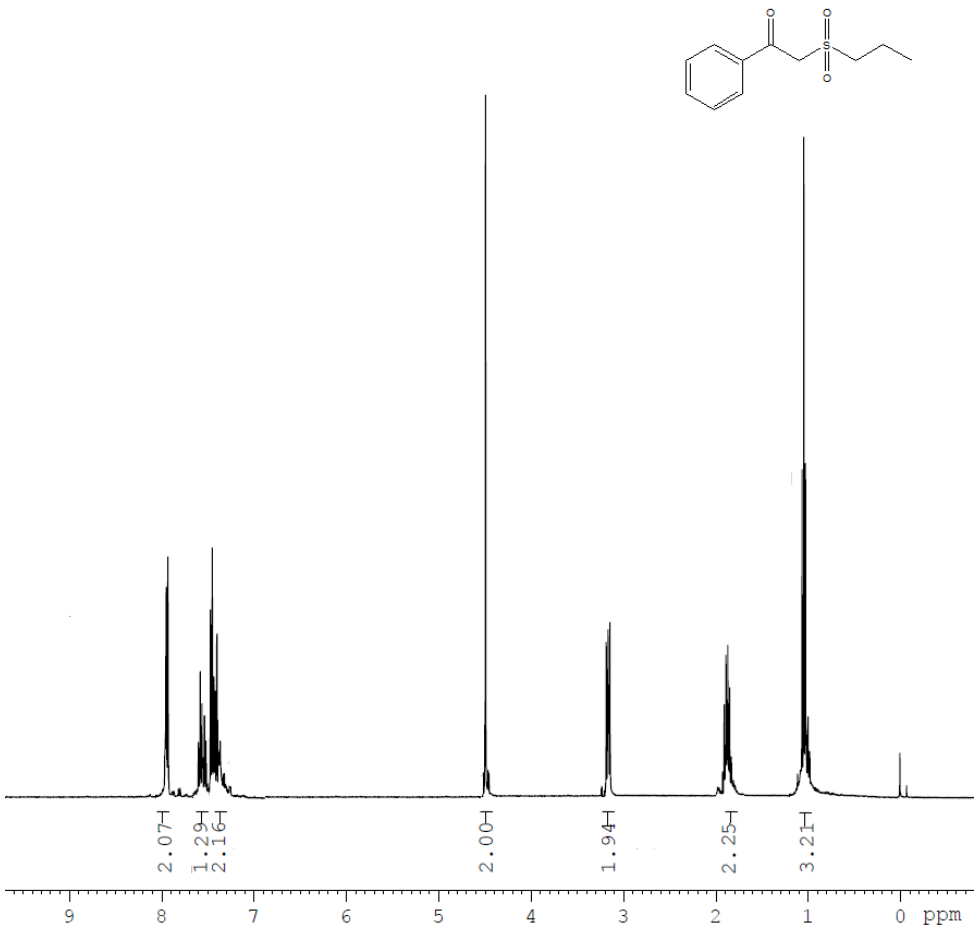

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

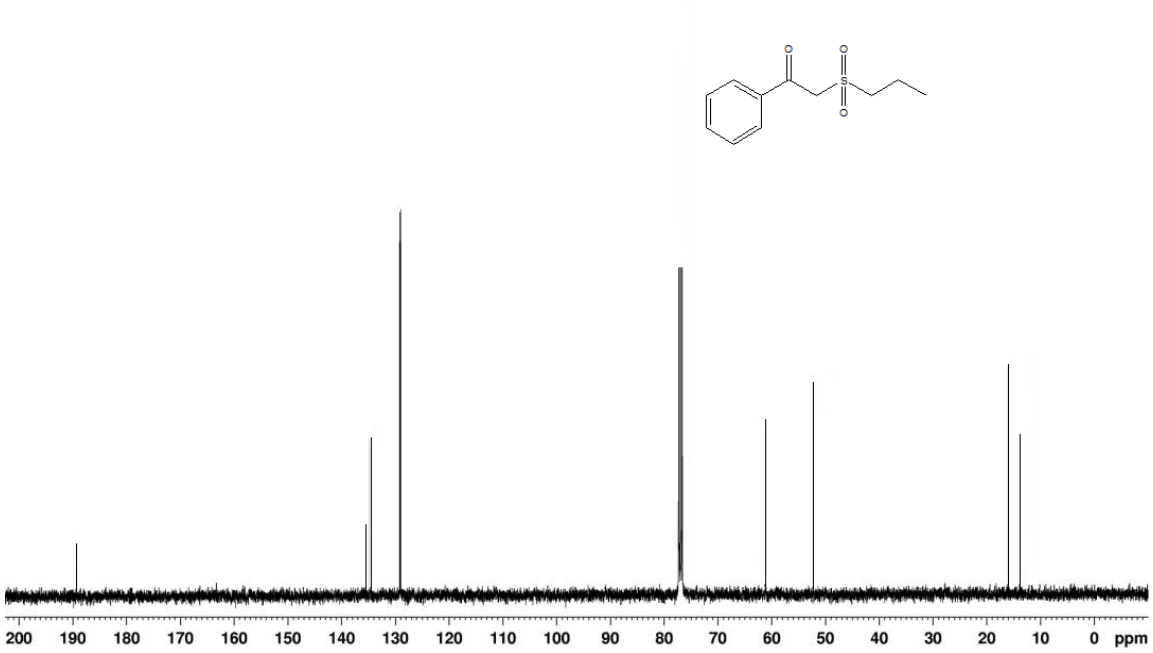

4.03
1.03
2.00
2.00
2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

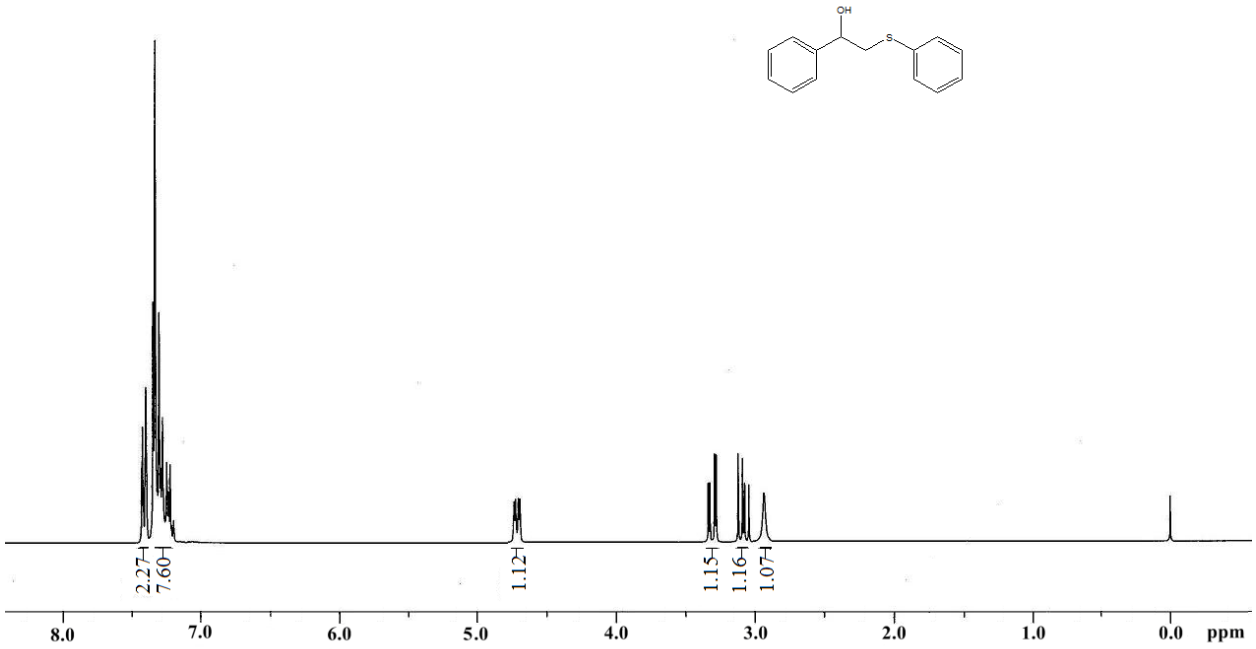

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

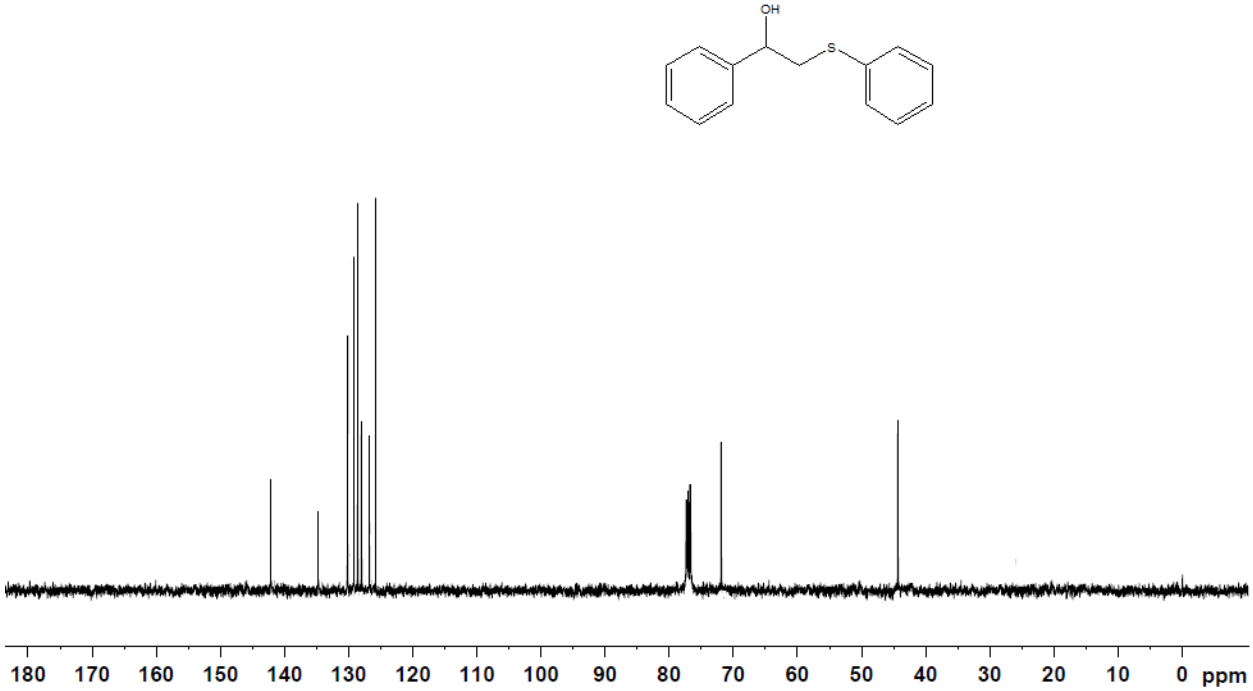

1.01
6.06
1.00
2.00
2.08
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

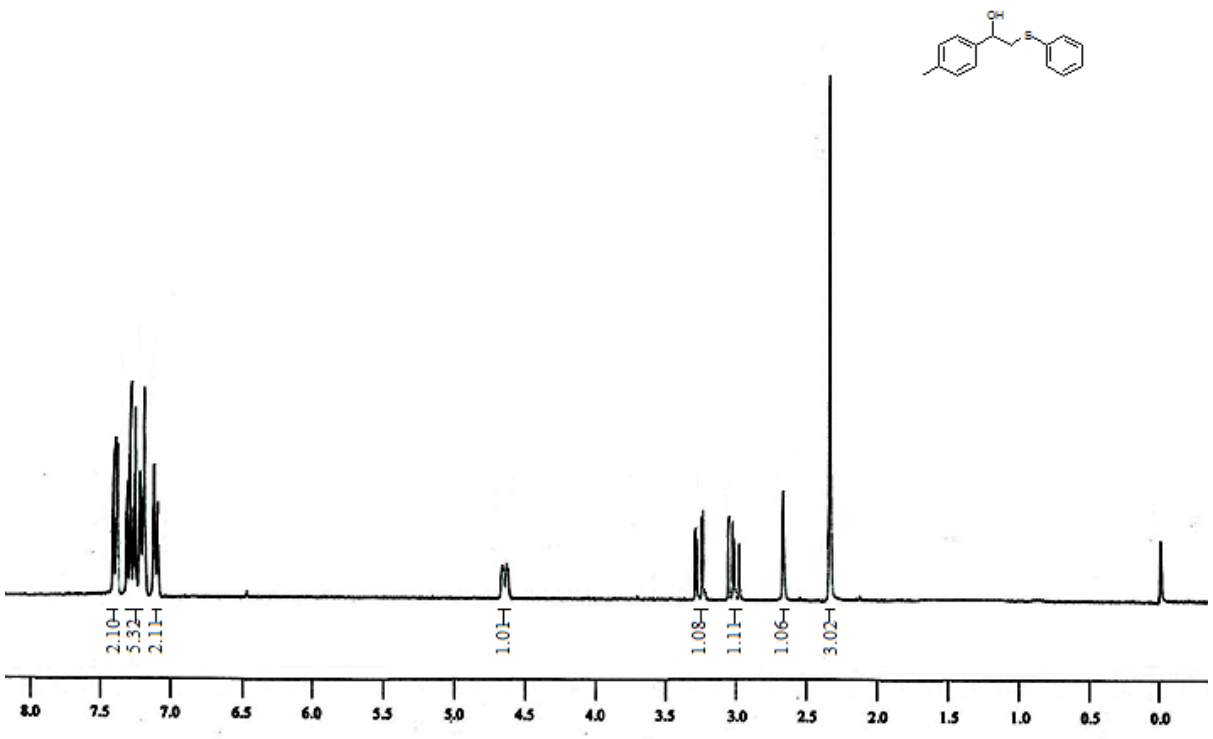

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

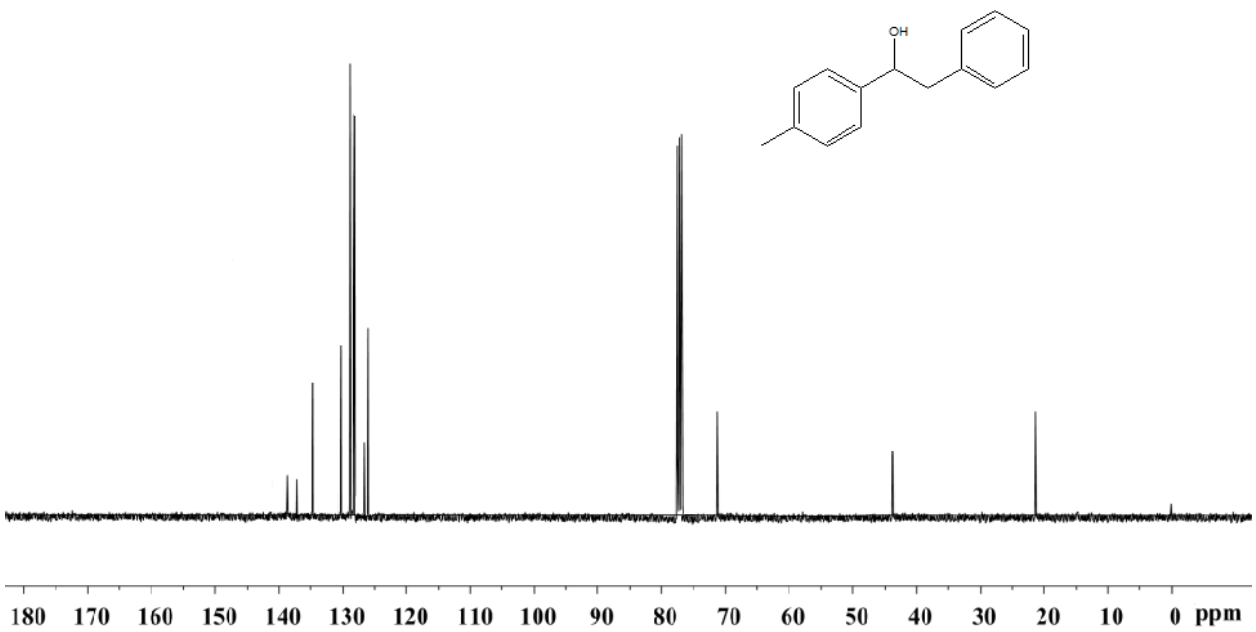

2.07
1.29
2.16
2.00
1.94
2.25
3.21
9
8
7
6
5
4
3
2
1
0
ppm

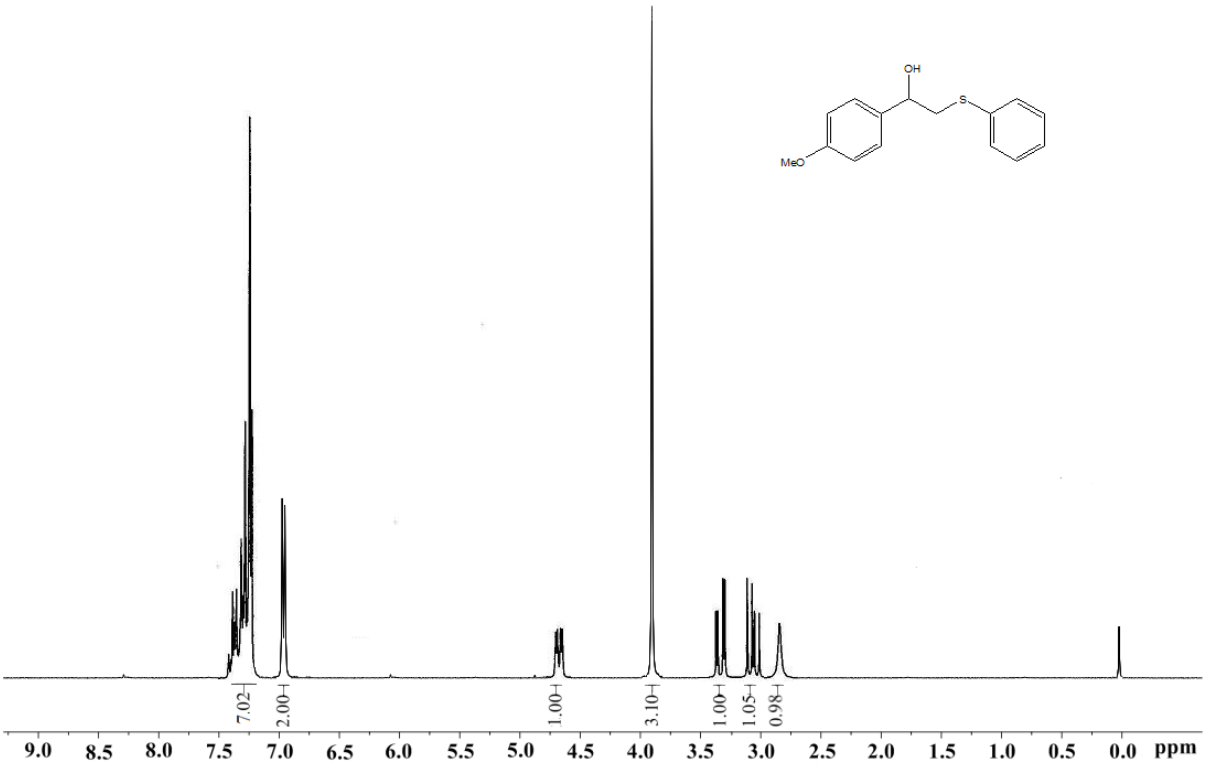

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

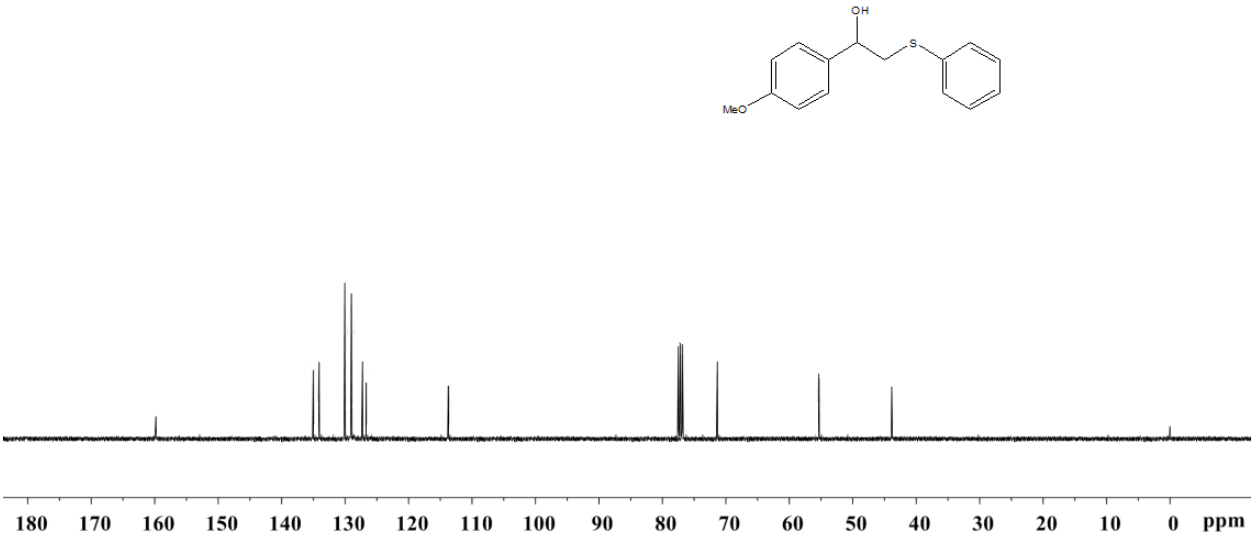

OH
S
2.27
7.60
1.12
1.15
1.16
1.07
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

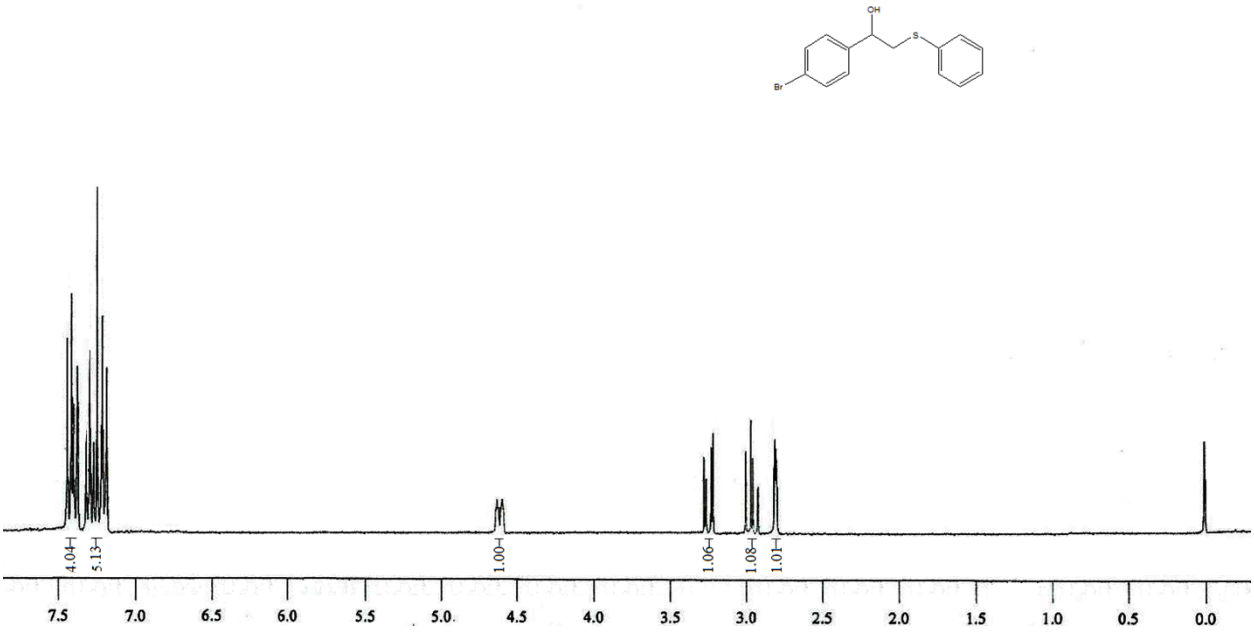

OH
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

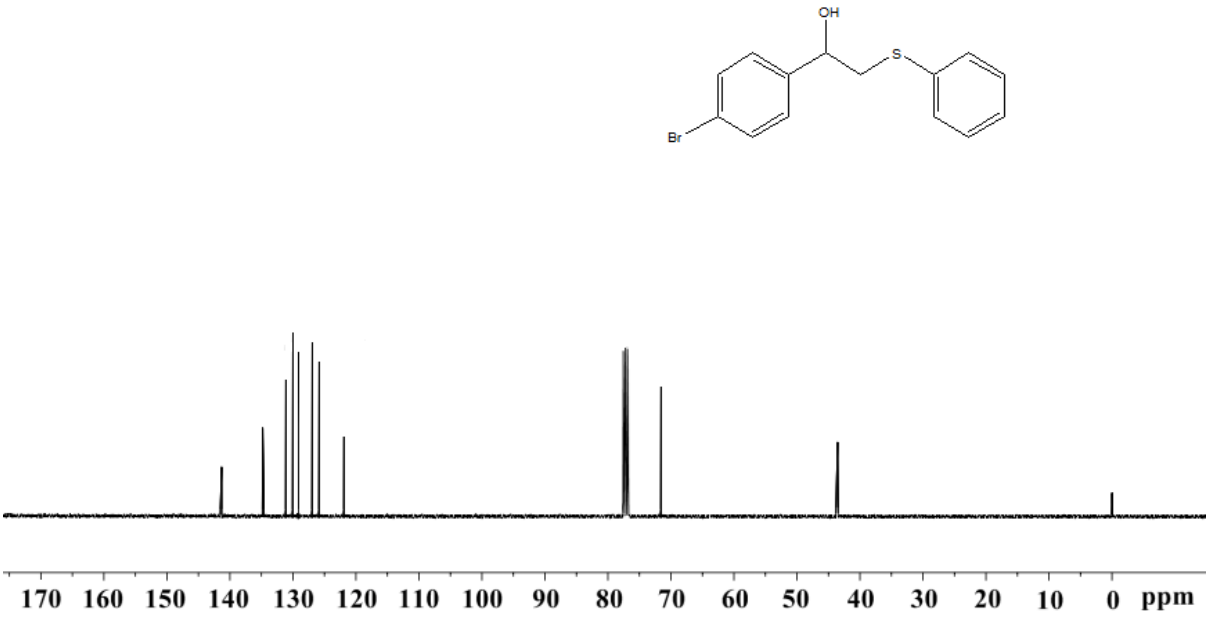

OH
S
2.10
5.32
2.11
1.01
1.08
1.11
1.06
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

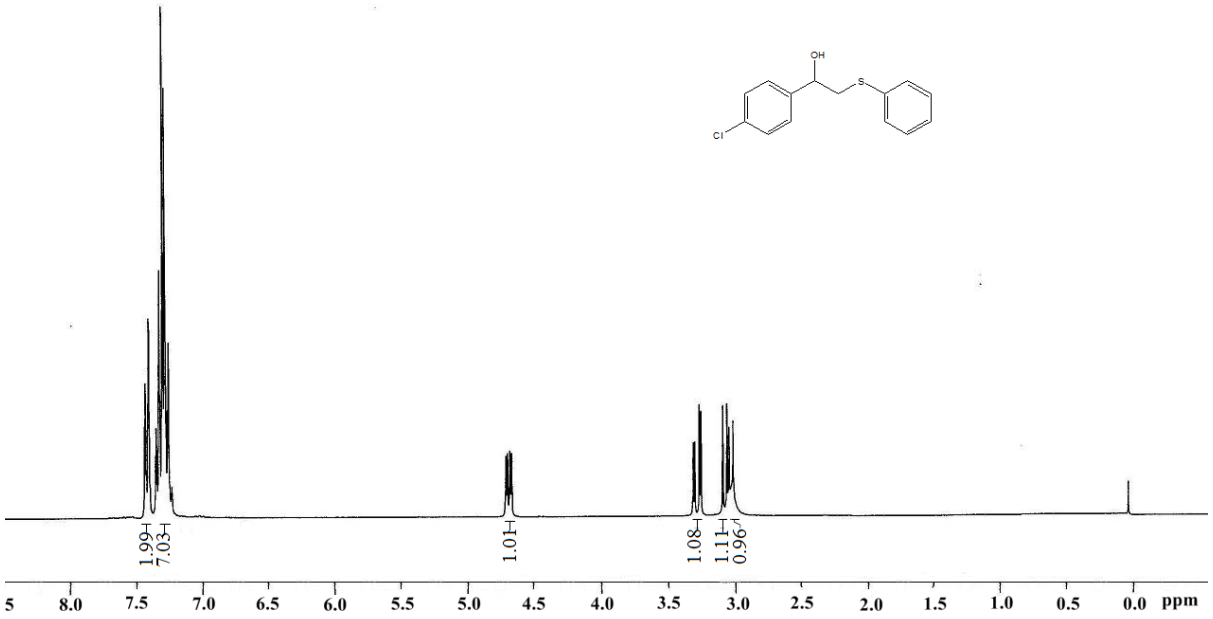

OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

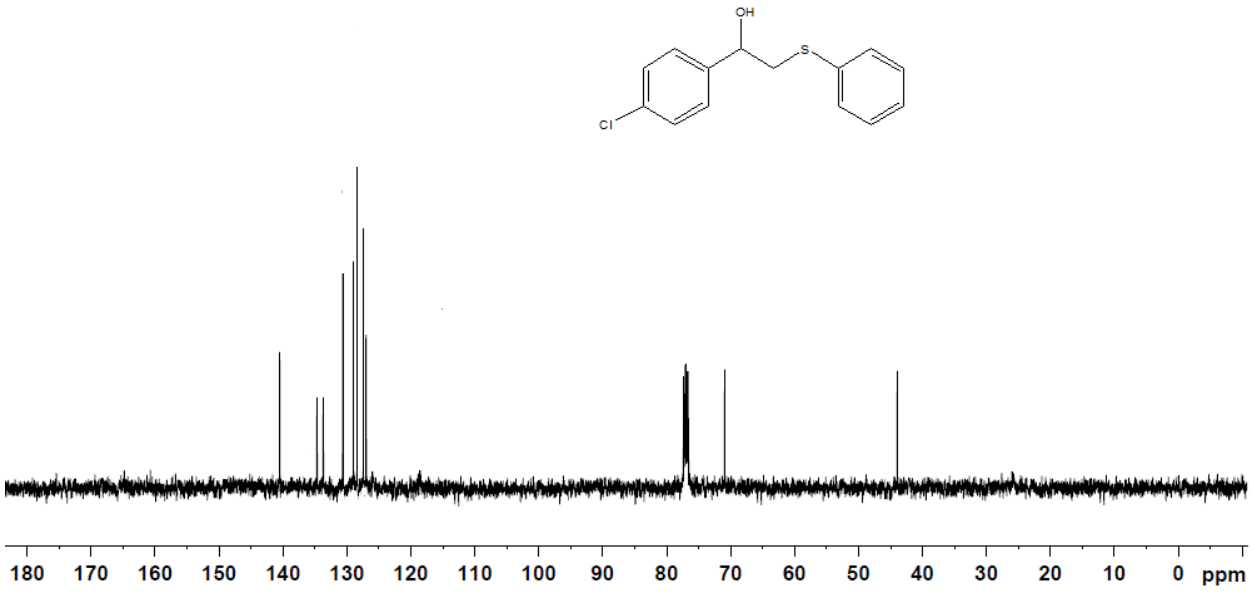

OH
S
MeO
7.02
2.00
1.00
3.10
1.00
1.05
0.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

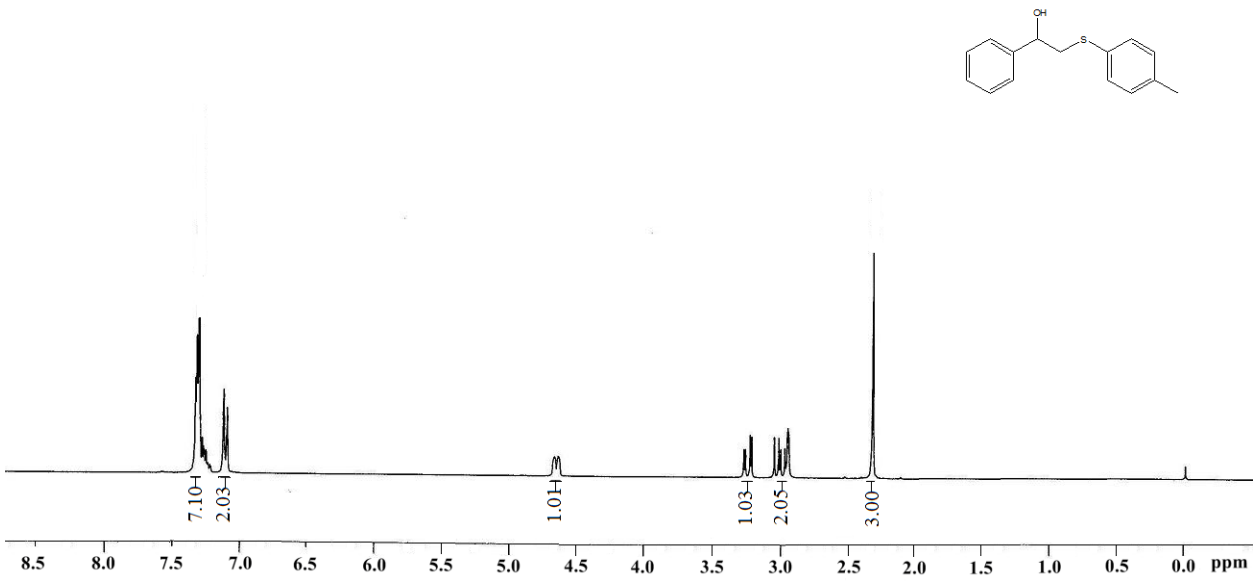

OH
S
MeO
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

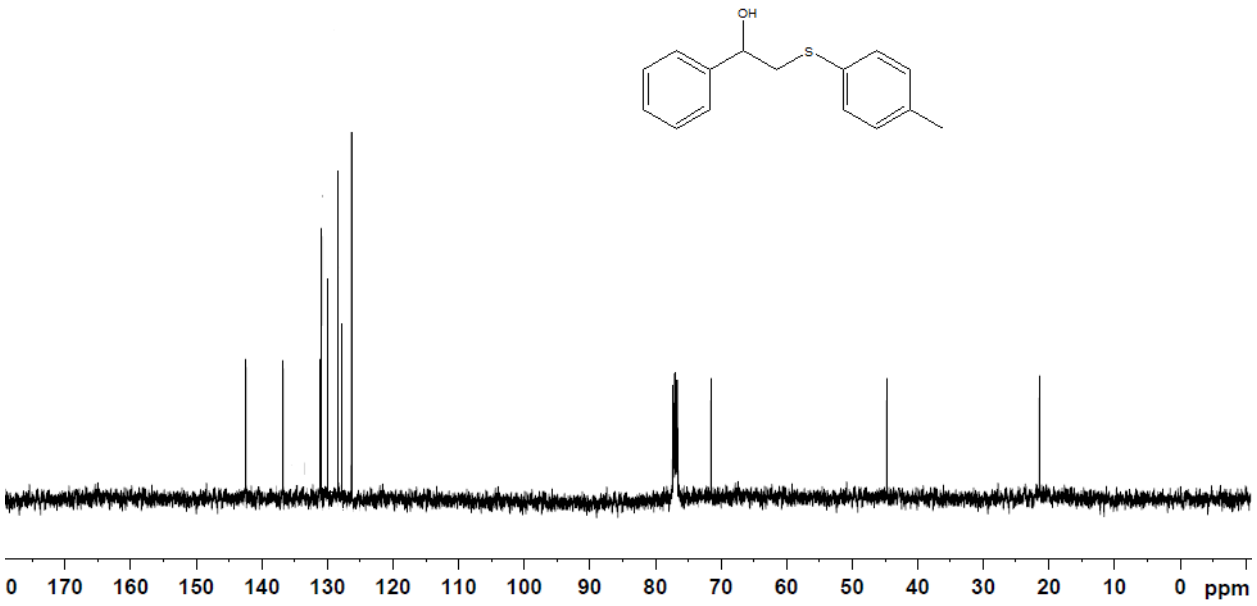

OH
S
Br
4.04
5.13
1.00
1.06
1.08
1.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

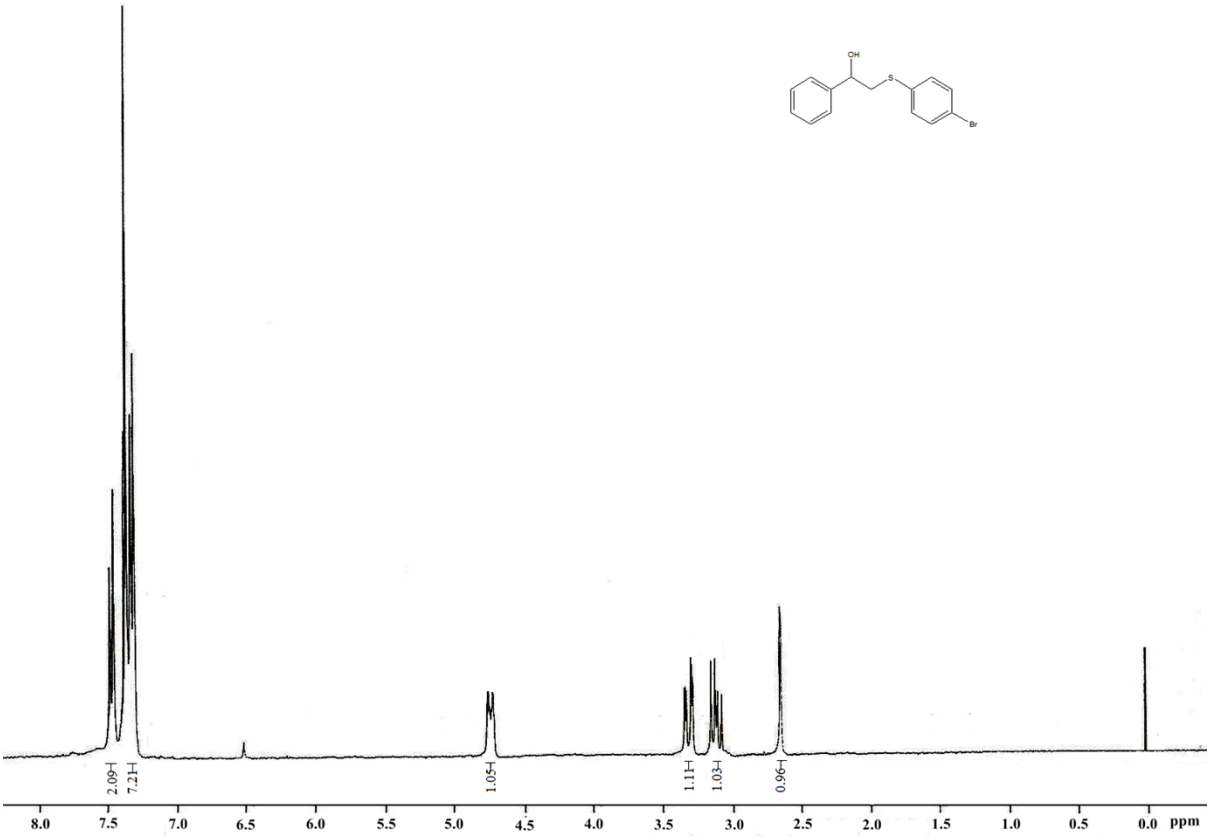

OH
S
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

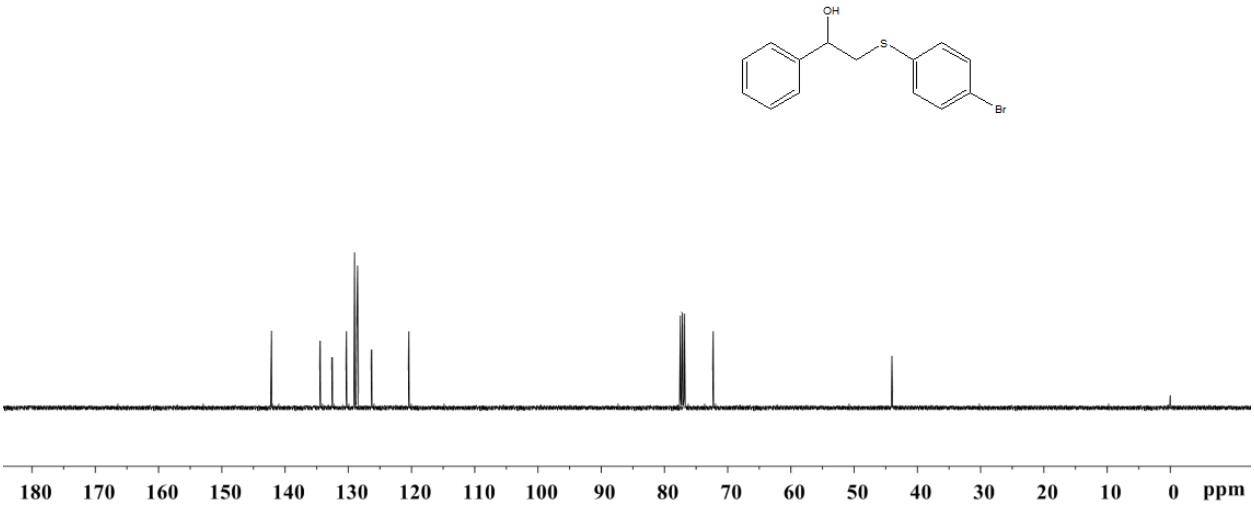

OH
S
Cl
1.99
7.03
1.01
1.08
1.11
0.96
5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

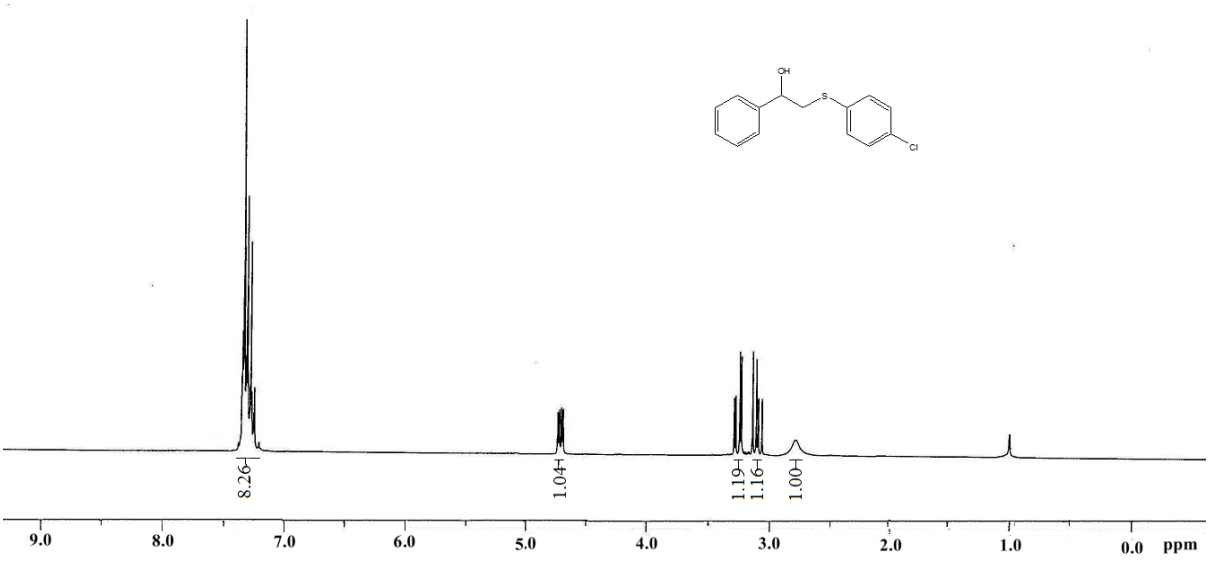

OH
S
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

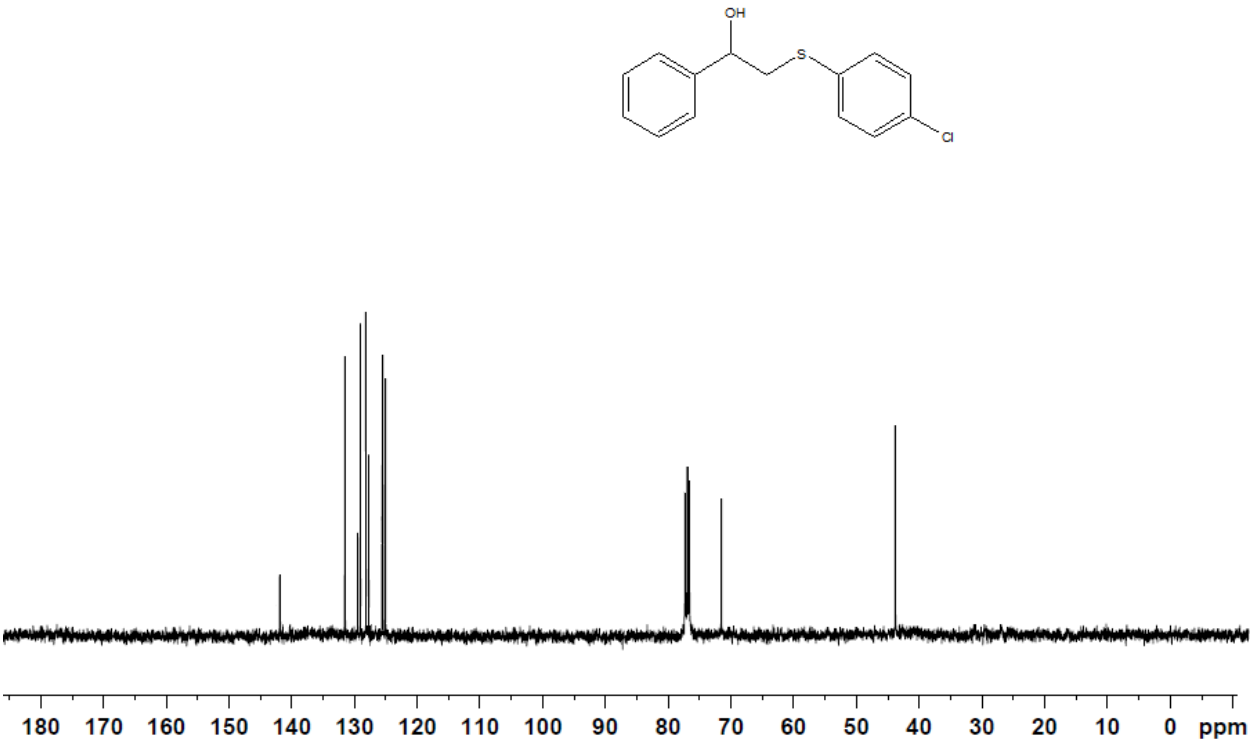

OH
S
7.10
2.03
1.01
1.03
2.05
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

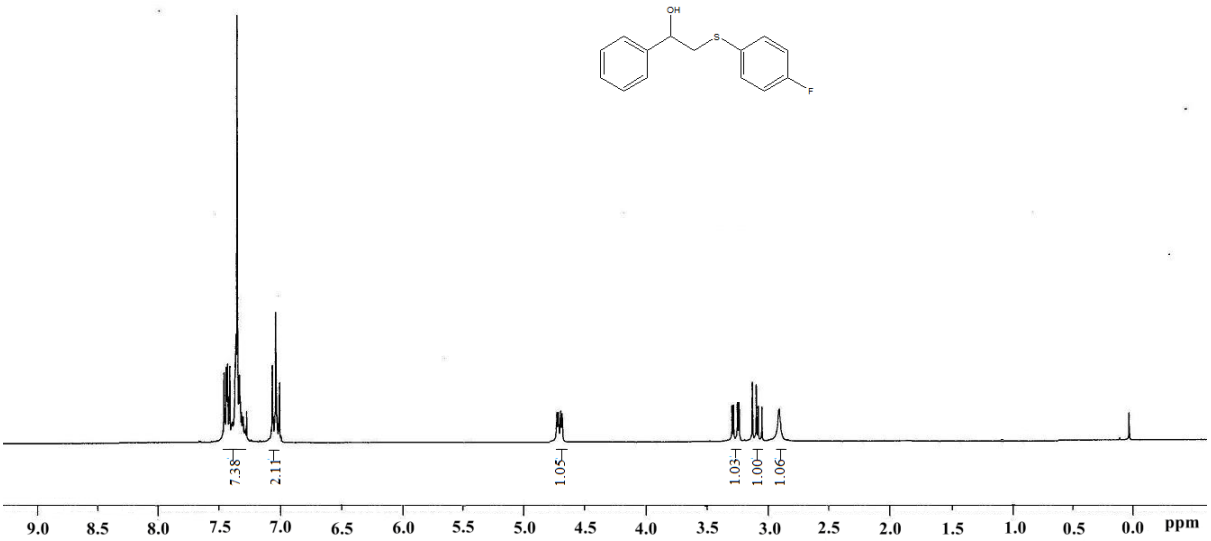

OH
S
0 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

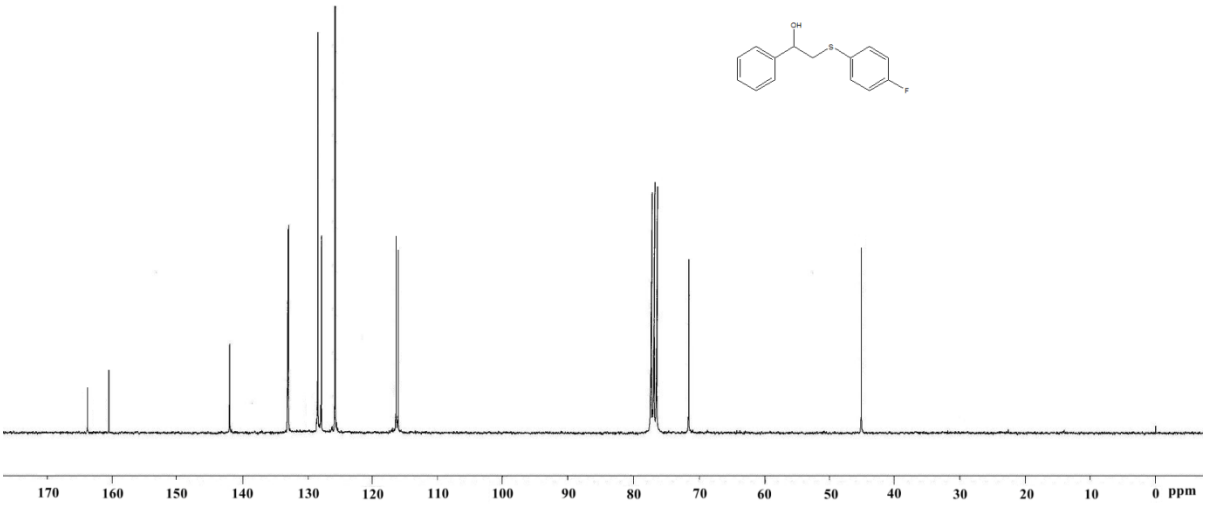

OH
S
Br
2.09
7.21
1.05
1.11
1.03
0.96
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

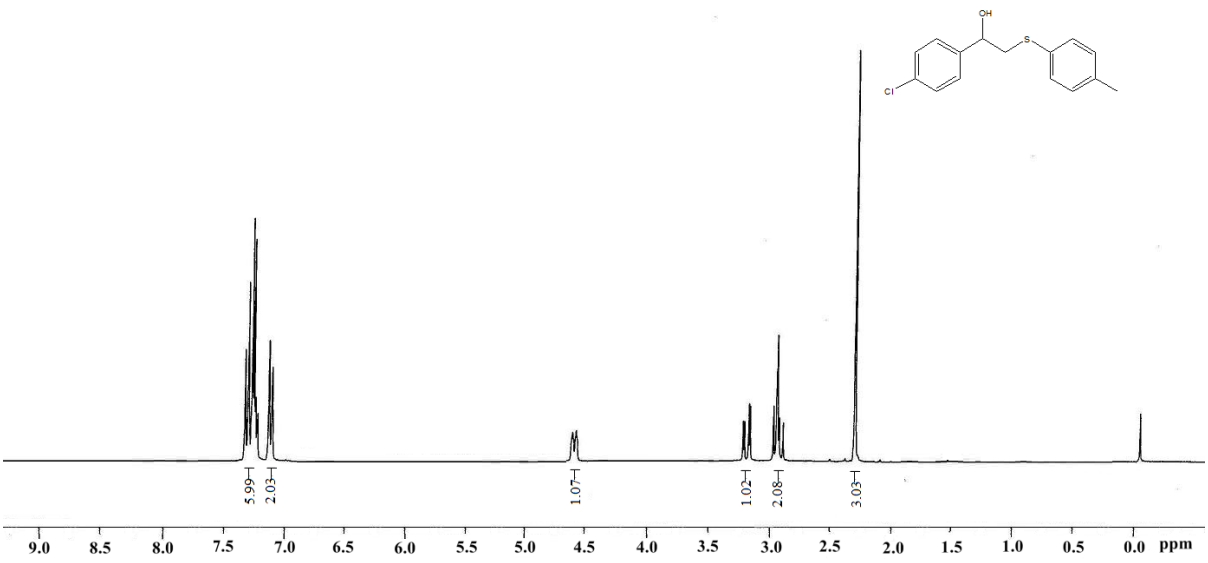

OH
S
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

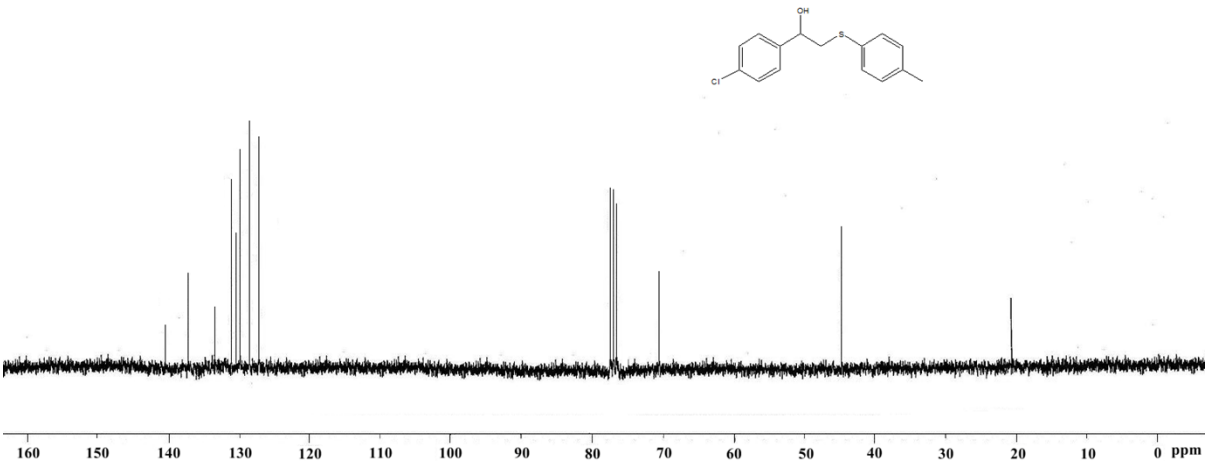

OH
S
Cl
8.26
1.04
1.19
1.16
1.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

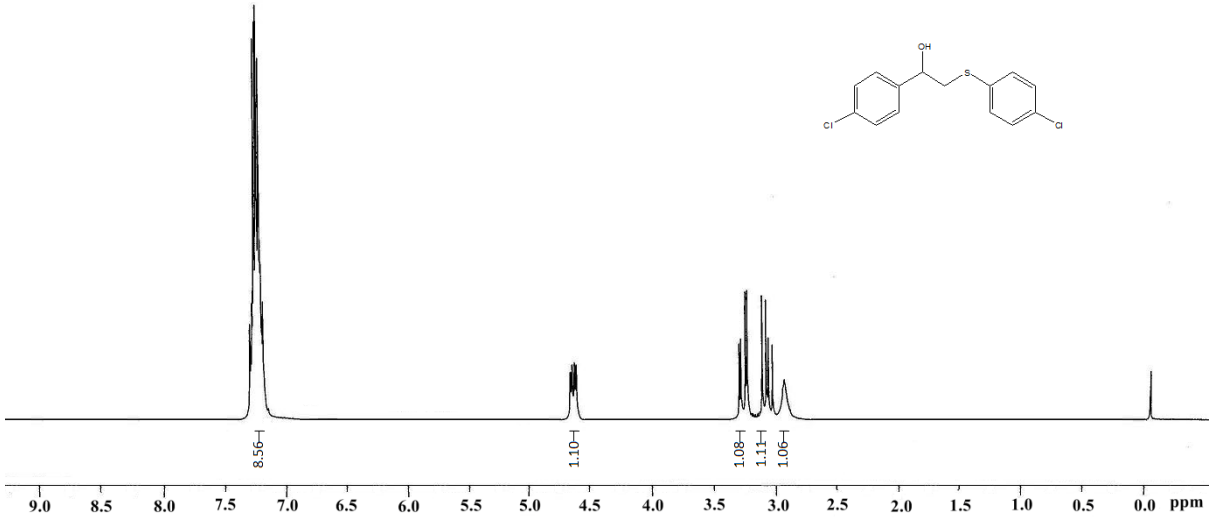

OH
S
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

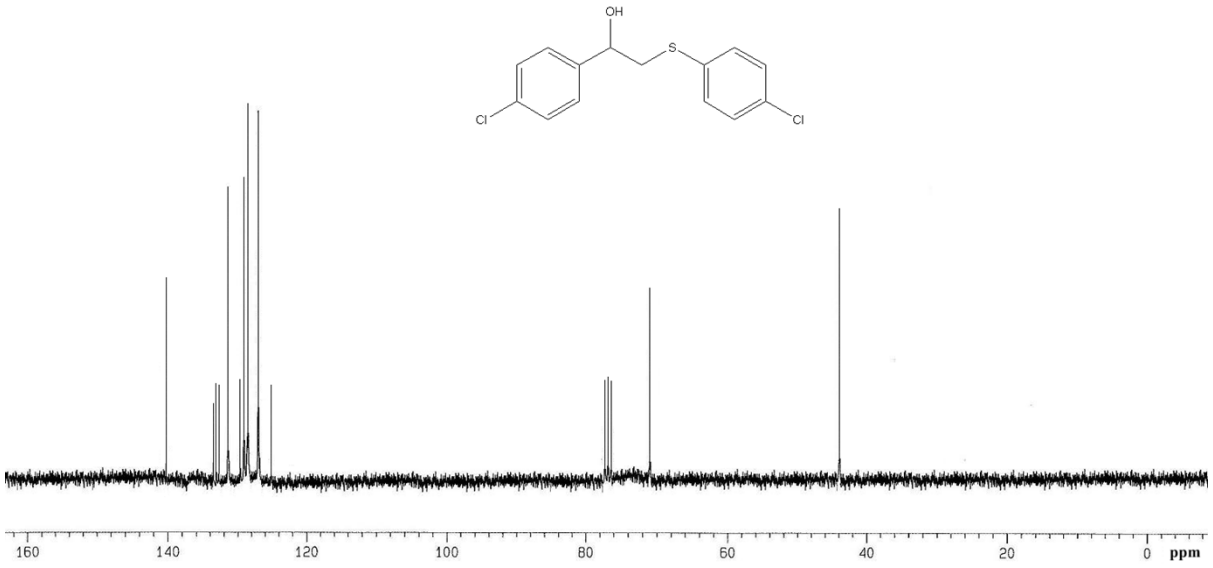

OH
S
F
7.38
2.11
1.05
1.03
1.00
1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

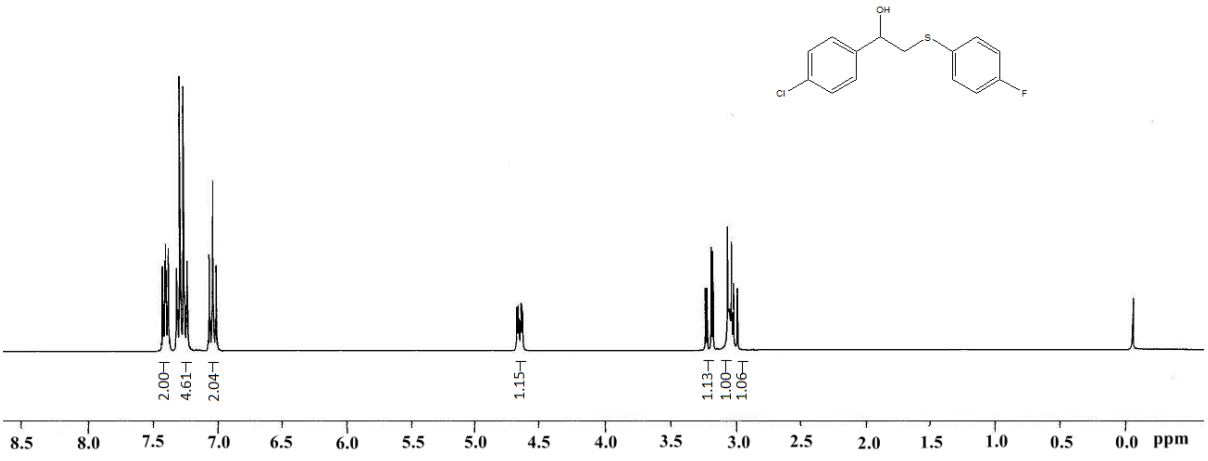

OH
S
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

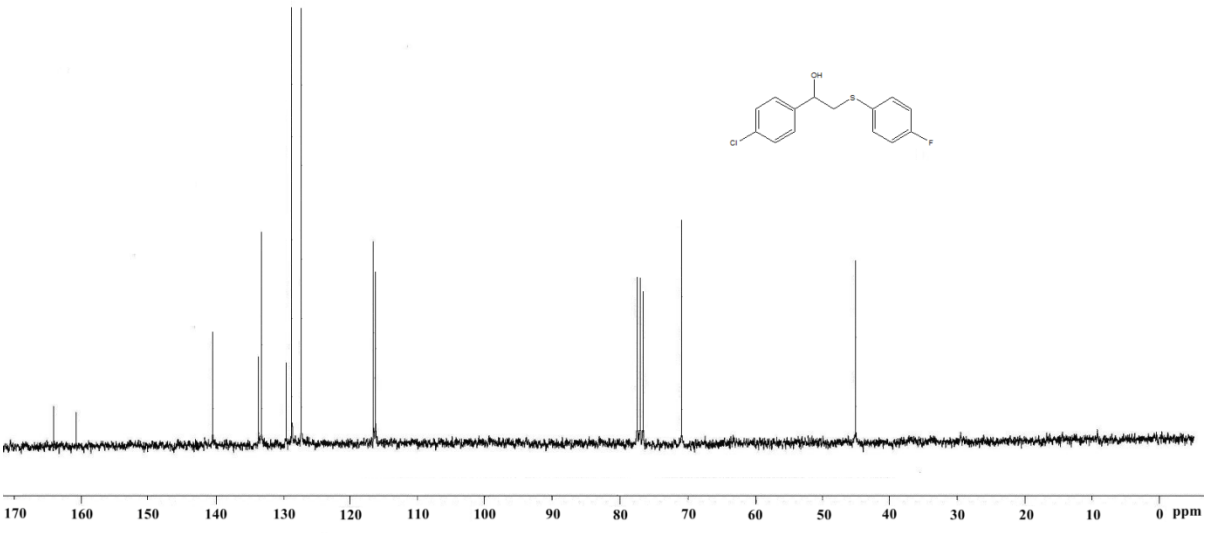

OH
S
Cl
5.99
2.03
1.07
1.02
2.08
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

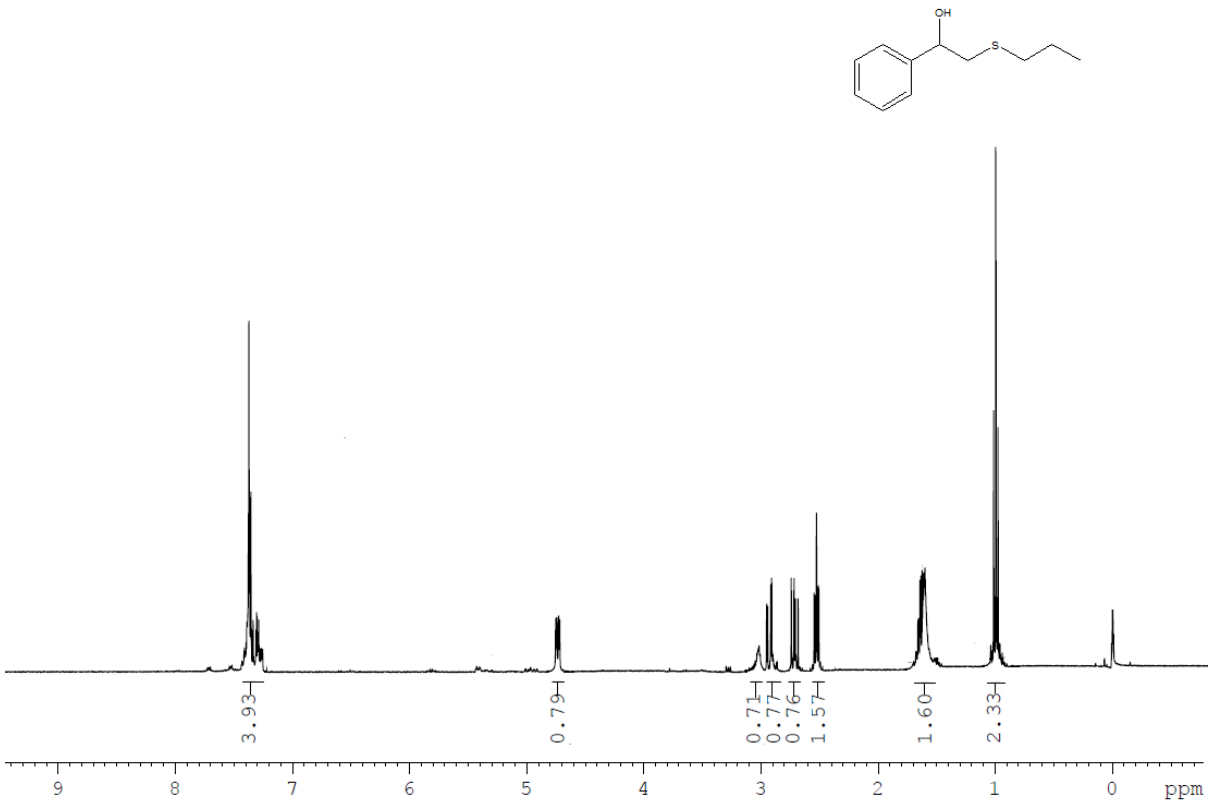

OH
S
Cl
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

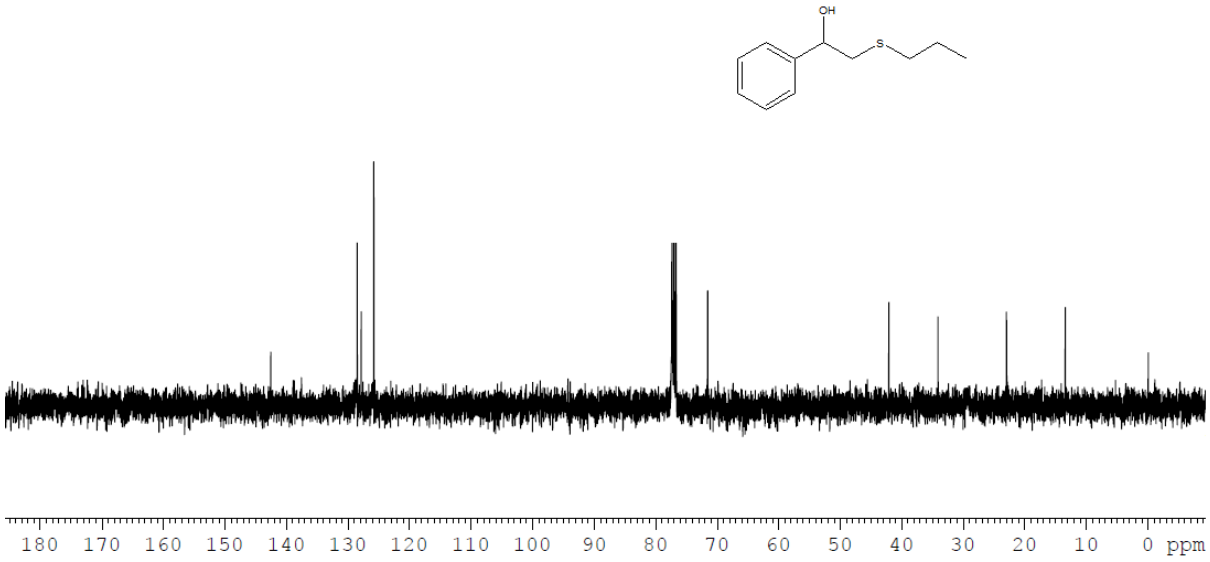

OH
S
Cl
Cl
8.56
1.10
1.08
1.11
1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


OH
S
Cl
Cl
160 140 120 100 80 60 40 20 0 ppm


OH
S
Cl
F
2.00
4.61
2.04
1.15
1.13
1.00
1.06
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 ppm


OH
S
Cl
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


OH
S
3.93
0.79
0.71
0.77
0.76
1.57
1.60
2.33
9
8
7
6
5
4
3
2
1
0
ppm


OH
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm