Supporting Information

Selective synthesis of sulfoxides and sulfones *via* controllable oxidation of sulfides with *N*-fluorobenzenesulfonimide

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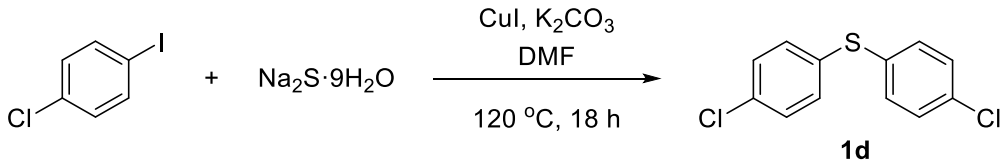
1. General Information

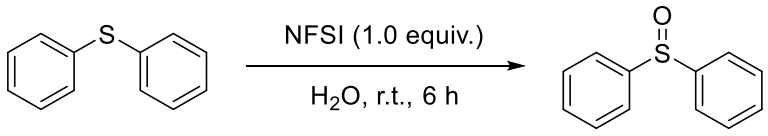
Unless otherwise noted, reactions were carried out in oven-dried glassware or sealed tube under ambient atmosphere. *N*, *N*-Dimethylformamide (DMF) was distilled from calcium hydride. Tetrahydrofuran (THF) was dried and distilled from sodium. Reactions were monitored by analytical thin-layer chromatography (TLC) on Merck silica gel 60 F_{254} plates (0.25 mm), visualized by ultraviolet light (254 nm) or by staining with ceric ammonium molybdate. ^{1}H NMR spectra were obtained on a Bruker AVANCE 400 MHz spectrometer at ambient temperature. Data were reported as follows: chemical shift on the δ scale using residual proton solvent as internal standard [δ 7.26 ($CHCl_3$); δ 2.50 (DMSO); δ 4.79 (H_2O); TMS: 0.00 ppm], multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets), integration, and coupling constant (J) in hertz (Hz). ^{13}C NMR spectra were obtained with proton decoupling on a Bruker AVANCE (100 MHz) spectrometer and were reported in ppm with residual solvent for internal standard [δ 77.0 ($CHCl_3$); δ 39.52 (DMSO)]. High resolution mass spectra were obtained on a Bruker SolariX 7.0T spectrometer. NCS = *N*-Chlorosuccinimide, NFSI = *N*-Fluorobenzenesulfonimide, TEMPO = 2,2,6,6-Tetramethylpiperidinooxy.

2. Experimental procedures



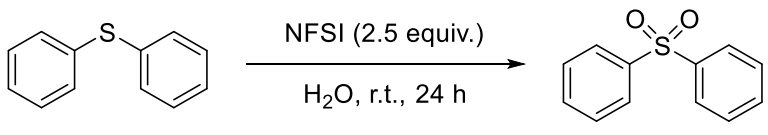
1d

General procedure for substrates[1]: A flame-dried test tube containing a magnetic stirring bar was charged with CuI (0.2 mmol), K_2CO_3 (2 mmol), $Na_2S·9H_2O$ (1.2 mmol), the 1-chloro-4-iodobenzene (2.0 mmol), and DMF (4 mL) under argon. The mixture was heated at 120 °C for 18 h and allowed to cool to room temperature. The resulting mixture was extracted with ethyl acetate (3×50 mL). The combined organic layers were dried with Na_2SO_4 and then concentrated under vacuum. The residue was purified by column chromatography on silica gel with an eluent consisting of petroleum ether and ethyl acetate.



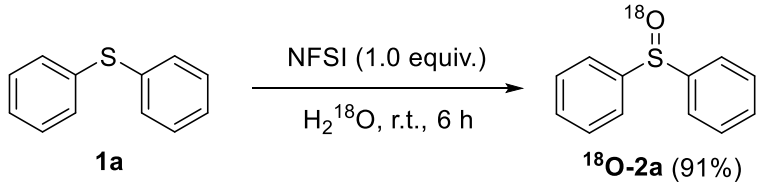
1a **2a**

General procedure for sulfoxides: To a solution of diphenyl sulfide **1a** (186 mg, 1.0 mmol) and NFSI (315 mg, 1.0 equiv.) in H_2O (2.0 mL) at room temperature. The resulting reaction mixture was stirred for 6 h and EtOAc (10 mL) was then added to the mixture. The resulting mixture was extracted with EtOAc (3×20 mL), and the combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by flash chromatography on silica gel to afford the desired product **2a** as a white solid (192 mg, 95% yield).

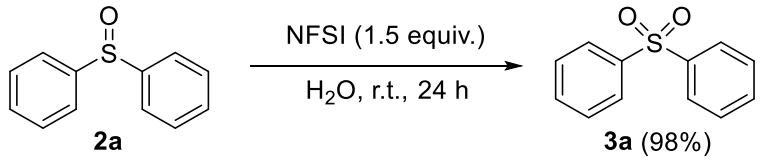


1a **3a**

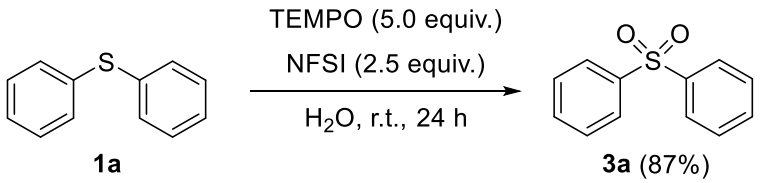
General procedure for sulfones: To a solution of diphenyl sulfide **1a** (186 mg, 1.0 mmol) and NFSI (788 mg, 2.5 equiv.) in H_2O (4.0 mL) at room temperature. The resulting reaction mixture was stirred for 24 h and EtOAc (10 mL) was then added to the mixture. The resulting mixture was extracted with EtOAc (3×20 mL), and the combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by flash chromatography on silica gel to afford the desired product **3a** as a white solid (200 mg, 92% yield).



Isotope labeling experiment with $H_2{}^{18}O$: To a solution of diphenyl sulfide **1a** (93 mg, 0.5 mmol) and NFSI (158 mg, 1.0 equiv.) in $H_2{}^{18}O$ (100 mg, 5.0 mmol) at room temperature. The resulting reaction mixture was stirred for 6 h and EtOAc (10 mL) was then added to the mixture. The resulting mixture was extracted with EtOAc (3×20 mL), and the combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by flash chromatography on silica gel to afford the desired product **^{18}O-2a** in 91% yield. HRMS of **^{18}O-2a**: calcd for $C_{12}H_{11}{}^{18}OS^+$ [M+H$^+$]: 205.0568; found: 205.0568.



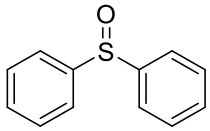
Intermediate probe experiment: To a solution of diphenyl sulfoxide **2a** (101 mg, 0.5 mmol) and NFSI (236 mg, 1.5 equiv.) in H_2O (2.0 mL) at room temperature. The resulting reaction mixture was stirred for 24 h and EtOAc (10 mL) was then added to the mixture. The resulting mixture was extracted with EtOAc (3×20 mL), and the combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by flash chromatography on silica gel to afford the desired product **3a** in 98% yield.



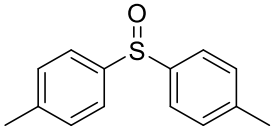
1a **3a** (87%)

Radical trapping experiments: To a solution of diphenyl sulfide **1a** (93 mg, 0.5 mmol), radical scavenger TEMPO (390 mg, 5.0 equiv.) and NFSI (394 mg, 2.5 equiv.) in H_2O (2.0 mL) at room temperature. The resulting reaction mixture was stirred for 24 h and EtOAc (10 mL) was then added to the mixture. The resulting mixture was extracted with EtOAc (3×20 mL), and the combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by flash chromatography on silica gel to afford the desired product **3a** in 87% yield.

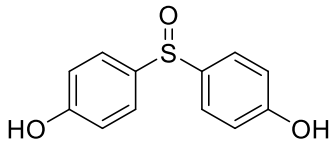
3. Characterization of Products



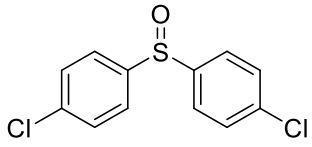
Sulfinyldibenzene (2a)[2]: Known compound. Isolated yield 95% (192 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.74-7.72 (m, 4H), 7.56-7.50 (m, 6H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 145.92, 131.06, 129.47, 124.08.



4,4'-Dimethyldiphenylsulfoxide (2b)[3]: Known compound. Isolated yield 94% (216 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.56 (d, J = 7.9 Hz, 4H), 7.33 (d, J = 7.9 Hz, 4H), 2.32 (s, 6H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 143.05, 141.01, 129.93, 124.16, 20.80.

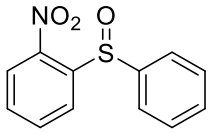


4,4'-Sulfinylbisphenol (2c)[3]: Known compound. Isolated yield 89% (208 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 10.09 (s, 2H, OH), 7.44-7.42 (m, 4H), 6.89-6.87 (m, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 159.86, 135.51, 126.50, 116.10.

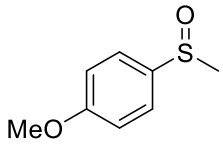


4,4'-Sulfinylbis(chlorobenzene) (2d)[3]: Known compound. Isolated yield 92% (248 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.77-7.75 (m, 4H), 7.64-7.62 (m, 4H);

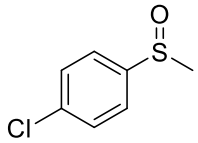
^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 144.52, 136.08, 129.67, 126.05.



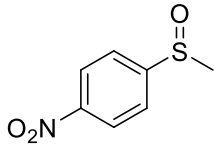
1-Nitro-2-(phenylsulfinyl)benzene (2e)[4]: Known compound. Isolated yield 85% (210 mg). ^{1}H NMR (CDCl$_3$, 400 MHz): δ (ppm) 8.60 (d, J = 7.9 Hz, 1H), 8.28 (d, J = 8.1 Hz, 1H), 8.03 (t, J = 7.6 Hz, 1H), 7.71 (dt, J = 8.6, 4.0 Hz, 3H), 7.42 (dd, J = 5.3, 1.9 Hz, 3H); ^{13}C NMR (CDCl$_3$, 100 MHz): δ (ppm) 145.08, 144.56, 143.84, 135.36, 131.54, 131.41, 129.25, 126.77, 126.28, 125.30.



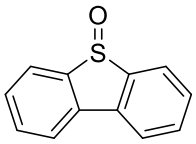
1-Methoxy-4-(methylsulfinyl)benzene (2f)[5]: Known compound. Isolated yield 90% (153 mg). ^{1}H NMR (CDCl$_3$, 400 MHz): δ (ppm) 7.59 (d, J = 8.6 Hz, 2H), 7.02 (d, J = 8.6 Hz, 2H), 3.85 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (CDCl$_3$, 100 MHz): δ (ppm) 161.85, 136.46, 125.35, 114.74, 55.42, 43.88.



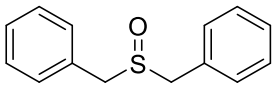
1-Chloro-4-(methylsulfinyl)benzene (2g)[2]: Known compound. Isolated yield 88% (153 mg). ^{1}H NMR (CDCl$_3$, 400 MHz): δ (ppm) 7.60 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.1 Hz, 2H), 2.73 (s, 3H); ^{13}C NMR (CDCl$_3$, 100 MHz): δ (ppm) 144.10, 137.22, 129.61, 124.95, 43.97.



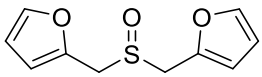
1-(Methylsulfinyl)-4-nitrobenzene (2h)[2]: Known compound. Isolated yield 83% (154 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.40 (d, J = 8.5 Hz, 2H), 7.85 (d, J = 8.6 Hz, 2H), 2.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 152.99, 149.56, 124.79, 124.56, 43.77.



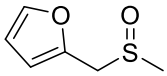
Dibenzothiophene-5-oxide (2i)[6]: Known compound. Isolated yield 87% (174 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 8.00 (d, J = 7.6 Hz, 2H), 7.82 (d, J = 7.7 Hz, 2H), 7.61 (t, J = 7.5 Hz, 2H), 7.51 (t, J = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 145.04, 136.99, 132.46, 129.45, 127.42, 121.83.



(Sulfinylbis(methylene))dibenzene (2j)[4]: Known compound. Isolated yield 95% (218 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 7.40-7.26 (m, 10H), 3.94-3.86 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 130.07 (2C), 128.89, 128.29, 57.20.

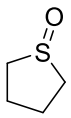


Difurfuryl sulfoxide (2k)[7]: Known compound. Isolated yield 92% (193 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 7.71 (s, 2H), 6.49-6.47 (m, 4H), 4.29 (d, J = 14.1 Hz, 2H), 4.07 (d, J = 14.1 Hz, 2H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 145.35, 143.83, 111.16, 111.06, 49.53.

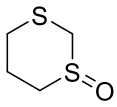


2-((Methylsulfinyl)methyl)furan (2l)[3]: Known compound. Isolated yield 87% (125 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 7.69 (s, 1H), 6.49-6.43 (m, 2H), 4.22 (d,

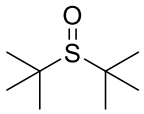
J = 14.0 Hz, 1H), 4.08 (d, *J* = 14.0 Hz, 1H), 2.52 (s, 3H).



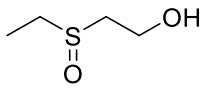
Tetramethylene sulfoxide (2m)[8]: Known compound. Isolated yield 94% (98 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.87-2.74 (m, 4H), 2.43-2.34 (m, 2H), 2.02-1.92 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 54.34, 25.32.



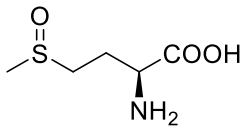
1,3-Dithiane 1-oxide (2n)[9]: Known compound. Isolated yield 95% (129 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 4.00 (d, *J* = 12.7 Hz, 1H), 3.64 (d, *J* = 12.7 Hz, 1H), 3.33-3.31 (m, 1H), 2.68-2.48 (m, 4H), 2.25-2.19 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 52.79, 50.35, 28.22, 27.08.



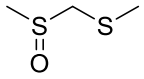
2-(Tert-butylsulfinyl)-2-methylpropane (2o)[6]: Known compound. Isolated yield 72% (117 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 1.24 (s, 18H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 56.88, 25.44.



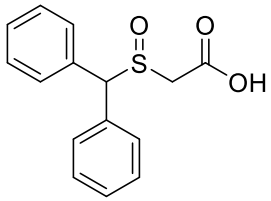
Ethyl 2-hydroxyethyl sulfoxide (2p)[10]: Known compound. Isolated yield 99% (120 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 4.16-4.07 (m, 2H), 2.95-2.78 (m, 4H), 1.34 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 55.40, 53.51, 45.67, 6.67.



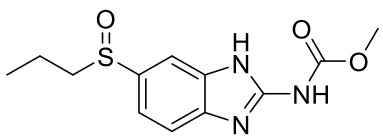
***L*-methionine sulfoxide (2q)**[5]: Known compound. Isolated yield 76% (125 mg). ^{1}H NMR (D_2O, 400 MHz): δ (ppm) 3.87 (td, J = 8.0, 7.3, 5.7 Hz, 1H), 3.06-2.97 (m, 2H), 2.74 (s, 3H), 2.31 (td, J = 8.0, 6.4 Hz, 2H); ^{13}C NMR (D_2O, 100 MHz): δ (ppm) 173.16, 53.29, 48.22, 36.52, 23.73.



Methyl((methylsulfinyl)methyl)sulfane (2r)[11]: Known compound. Isolated yield 97% (120 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 3.98 (d, J = 13.5 Hz, 1H), 3.78 (d, J = 13.6 Hz, 1H), 2.59 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 55.21, 37.21, 16.38.

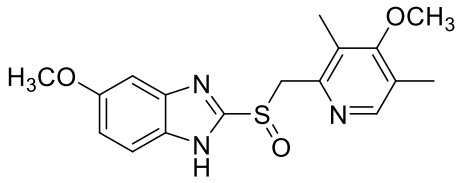


2-Benzhydrylsulphinylacetic acid (2s)[12]: Known compound. Isolated yield 71% (195 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 13.20 (s, 1H, COOH), 7.52 (dt, J = 6.9, 1.5 Hz, 4H), 7.45-7.36 (m, 6H), 5.41 (s, 1H), 3.57 (d, J = 14.0 Hz, 1H), 3.32 (d, J = 14.0 Hz, 1H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 167.38, 136.62, 134.88, 129.61, 129.12, 128.58, 128.52, 128.12, 128.06, 69.27, 55.42.

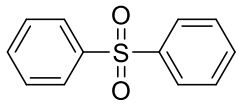


Ricobendazole (2t)[6]: Known compound. Isolated yield 52% (146 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 11.87 (s, 2H), 7.71 (s, 1H), 7.57 (d, J = 8.2 Hz, 1H), 7.33

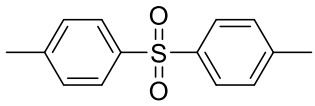
(dt, *J* = 8.4, 1.4 Hz, 1H), 3.79 (s, 3H), 2.88-2.74 (m, 2H), 1.61 (dt, *J* = 14.7, 7.3 Hz, 1H), 1.49 (tt, *J* = 14.0, 9.1 Hz, 1H), 0.95 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 154.41, 148.64, 136.18, 116.79, 58.22, 52.64, 15.44, 12.98.



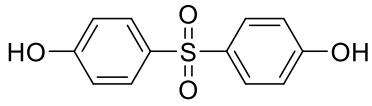
Omeprazole (2u)[6]: Known compound. Isolated yield 46% (159 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 13.44 (s, 1H), 8.19 (s, 1H), 7.57 (s, 1H), 7.04 (s, 1H), 6.93 (d, *J* = 8.9 Hz, 1H), 4.77 (d, *J* = 13.6 Hz, 1H), 4.69 (d, *J* = 13.5 Hz, 1H), 3.81 (s, 3H), 3.69 (s, 3H), 2.19 (d, *J* = 13.2 Hz, 6H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 163.98, 157.44, 156.43, 153.03, 150.09, 149.61, 137.96, 135.95, 126.95, 125.98, 120.89, 114.75, 113.35, 101.94, 95.04, 60.55, 60.17, 55.94, 13.36, 11.56.



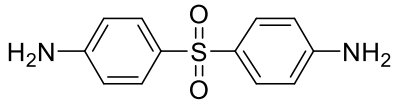
Diphenyl sulfone (3a)[2]: Known compound. Isolated yield 93% (203 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 7.98-7.96 (m, 4H), 7.72-7.61 (m, 6H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 141.11, 133.67, 129.72, 127.33.



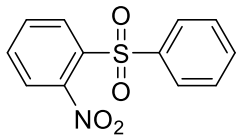
4,4'-Sulfonylbis(methylbenzene) (3b)[13]: Known compound. Isolated yield 96% (236 mg). ^{1}H NMR (d^6-DMSO, 400 MHz): δ (ppm) 7.81 (d, *J* = 8.0 Hz, 4H), 7.40 (d, *J* = 8.0 Hz, 4H), 2.36 (s, 6H); ^{13}C NMR (d^6-DMSO, 100 MHz): δ (ppm) 144.07, 138.63, 130.09, 127.21, 20.95.



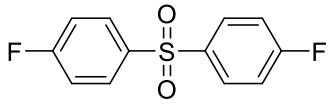
4,4'-Sulfonyldiphenol (3c)[3]: Known compound. Isolated yield 92% (230 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 10.53 (s, 2H), 7.70 (d, J = 8.8 Hz, 4H), 6.89 (d, J = 8.8 Hz, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 161.66, 132.18, 129.42, 116.02.



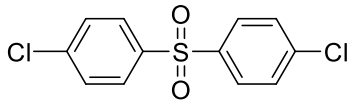
4,4'-Sulfonyldianiline (3d)[14]: Known compound. Isolated yield 86% (213 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.44 (d, J = 8.4 Hz, 4H), 6.57 (d, J = 8.5 Hz, 4H), 5.99 (s, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 152.75, 128.60, 128.18, 112.90.



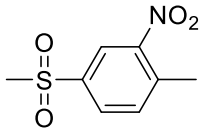
1-Nitro-2-(phenylsulfonyl)benzene (3e)[15]: Known compound. Isolated yield 82% (216 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 8.41-8.39 (m, 1H), 8.05-7.97 (m, 5H), 7.78-7.68 (m, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 147.80, 139.97, 135.96, 134.34, 133.29, 132.43, 131.50, 129.63, 127.69, 124.92.



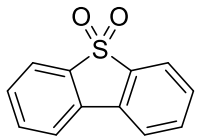
4,4'-Sulfonylbis(fluorobenzene) (3f)[13]: Known compound. Isolated yield 80% (203 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 8.07 (dd, J = 8.6, 5.2 Hz, 4H), 7.47 (t, J = 8.6 Hz, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 164.93 (d, J = 252.36 Hz), 137.34 (d, J = 3.11 Hz), 130.62 (d, J = 9.34 Hz), 116.99 (d, J = 23,24 Hz).



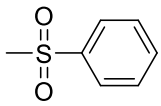
4,4'-Dichlorodiphenyl sulfone (3g)[3]: Known compound. Isolated yield 78% (223 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 8.00 (d, J = 8.4 Hz, 4H), 7.71 (d, J = 8.4 Hz, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 139.45, 139.07, 129.95, 129.40.



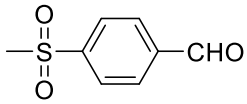
2-Nitro-4-methylsulfonyltoluene (3h)[16]: Known compound. Isolated yield 77% (166 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 8.47 (d, J = 1.7 Hz, 1H), 8.16 (dt, J = 8.2, 1.6 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 3.33 (s, 3H), 2.63 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 148.82, 139.74, 138.78, 134.22, 131.14, 123.35, 43.23, 19.61.



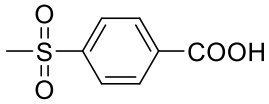
Dibenzo[b,d]thiophene 5,5-dioxide (3i)[6]: Known compound. Isolated yield 65% (140 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 8.21 (d, J = 7.7 Hz, 2H), 7.99 (d, J = 7.7 Hz, 2H), 7.82 (t, J = 7.6 Hz, 2H), 7.67 (t, J = 7.6 Hz, 2H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 136.95, 134.52, 130.92, 130.83, 122.67, 121.97.



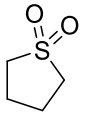
Methyl phenyl sulfone (3j)[2]: Known compound. Isolated yield 94% (147 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.96-7.94 (m, 2H), 7.77-7.65 (m, 3H), 3.37 (s, 0H), 3.23 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 140.84, 133.60, 129.41, 126.90, 43.51.



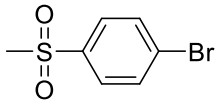
4-Methylsulphonyl benzaldehyde (3k)[17]: Known compound. Isolated yield 75% (138 mg). ^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm) 10.13 (s, 1H), 8.14-8.07 (m, 4H), 3.10 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 190.67, 145.31, 139.62, 130.35, 128.16, 44.24.



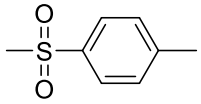
4-Methylsulphonylbenzoic acid (3l)[2]: Known compound. Isolated yield 79% (158 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 13.56 (s, 1H), 8.18 (d, J = 8.1 Hz, 2H), 8.06 (d, J = 8.1 Hz, 2H), 3.29 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 166.21, 144.35, 135.29, 130.26, 127.37, 43.30.



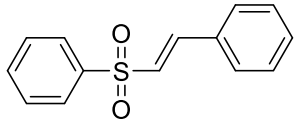
Tetrahydrothiophene 1,1-dioxide (3m)[8]: Known compound. Isolated yield 95% (114 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 3.02-2.98 (m, 4H), 2.10-2.06 (m, 4H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 50.58, 22.16.



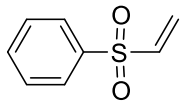
4-Bromophenyl methyl sulfone (3n)[2]: Known compound. Isolated yield 94% (220 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.89-7.87 (m, 4H), 3.25 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 140.04, 132.45, 129.05, 127.68, 43.39.



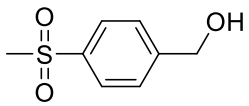
1-Methyl-4-(methylsulfonyl)-benzene (3o)[8]: Known compound. Isolated yield 97% (165 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.82 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 3.18 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 144.07, 138.07, 129.81, 126.94, 43.68, 21.01.



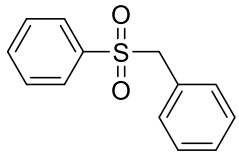
(*E*)-[2-(Phenylsulfonyl)vinyl]benzene (3p)[15]: Known compound. Isolated yield 95% (232 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.95 (d, *J* = 7.6 Hz, 2H), 7.77-7.61 (m, 7H), 7.44 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 142.04, 140.72, 133.58, 132.37, 131.17, 129.62, 129.01, 128.98, 128.06, 127.13.



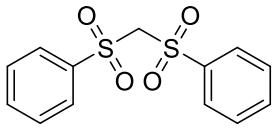
(Vinylsulfonyl)benzene (3q)[18]: Known compound. Isolated yield 83% (139 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.90-7.87 (m, 2H), 7.78-7.65 (m, 3H), 7.14 (dd, *J* = 16.4, 9.8 Hz, 1H), 6.36 (d, *J* = 16.4 Hz, 1H), 6.22 (d, *J* = 9.9 Hz, 1H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 139.50, 138.52, 133.83, 129.61, 128.71, 127.38.



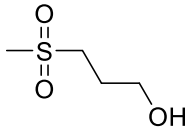
(4-(Methylsulfonyl)phenyl)methanol (3r)[17]: Known compound. Isolated yield 87% (162 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.88 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 5.46 (td, *J* = 5.8, 1.0 Hz, 1H), 4.62 (d, *J* = 5.7 Hz, 2H), 3.20 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 148.77, 139.09, 126.89, 126.87, 62.21, 43.69.



Benzylsulfonyl-benzene (3s)[2]: Known compound. Isolated yield 92% (213 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.71 (d, J = 7.4 Hz, 3H), 7.59 (t, J = 7.7 Hz, 2H), 7.30 (t, J = 7.4 Hz, 3H), 7.14 (dd, J = 7.6, 1.8 Hz, 2H), 4.68 (s, 2H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 138.33, 133.79, 130.96, 129.09, 128.65, 128.32, 128.20, 128.02, 60.69.



Bis(phenylsulfonyl)methane (3t)[19]: Known compound. Isolated yield 72% (213 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 7.90-7.88 (m, 4H), 7.76 (t, J = 7.5 Hz, 2H), 7.63 (t, J = 7.7 Hz, 4H), 5.94 (s, 2H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 138.85, 134.40, 129.15, 128.33, 71.83.



3-(Methylsulfonyl)propan-1-ol (3u)[20]: Known compound. Isolated yield 98% (135 mg). ^{1}H NMR (d^{6}-DMSO, 400 MHz): δ (ppm) 4.71-4.68 (t, J = 4.8 Hz, 1H), 3.49 (q, J = 5.8 Hz, 2H), 3.14-3.10 (dd, J = 10.4, 5.8 Hz, 2H), 2.97 (s, 3H), 1.86-1.79 (m, 2H); ^{13}C NMR (d^{6}-DMSO, 100 MHz): δ (ppm) 59.12, 51.07, 40.23, 25.42.

4. References

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Yu, X. Liu, L. Zhong, K. Leng, W. Huang, M. J. Koh, K. P. Loh, *Adv. Mater.,* 2020, **32**, 1906437.

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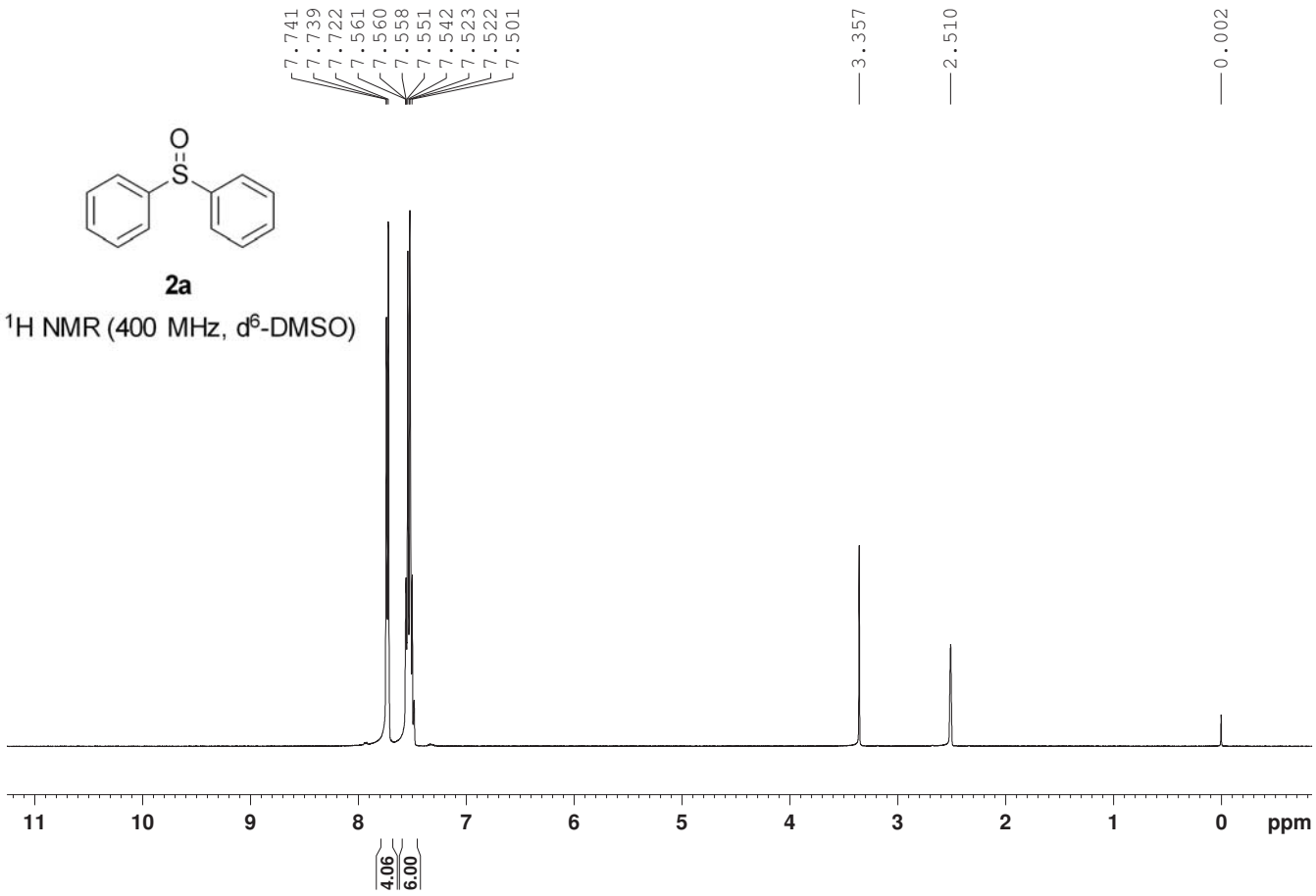
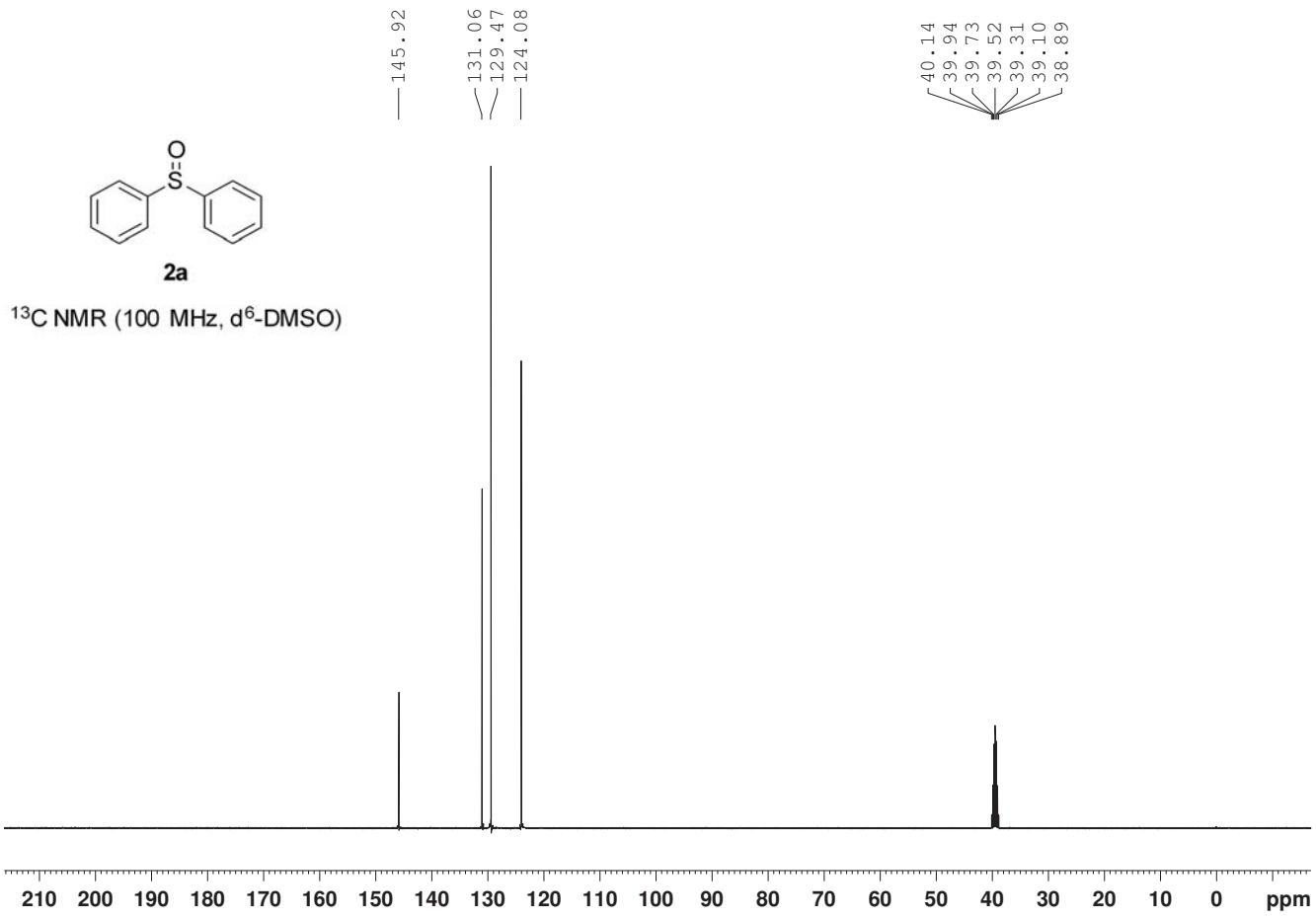
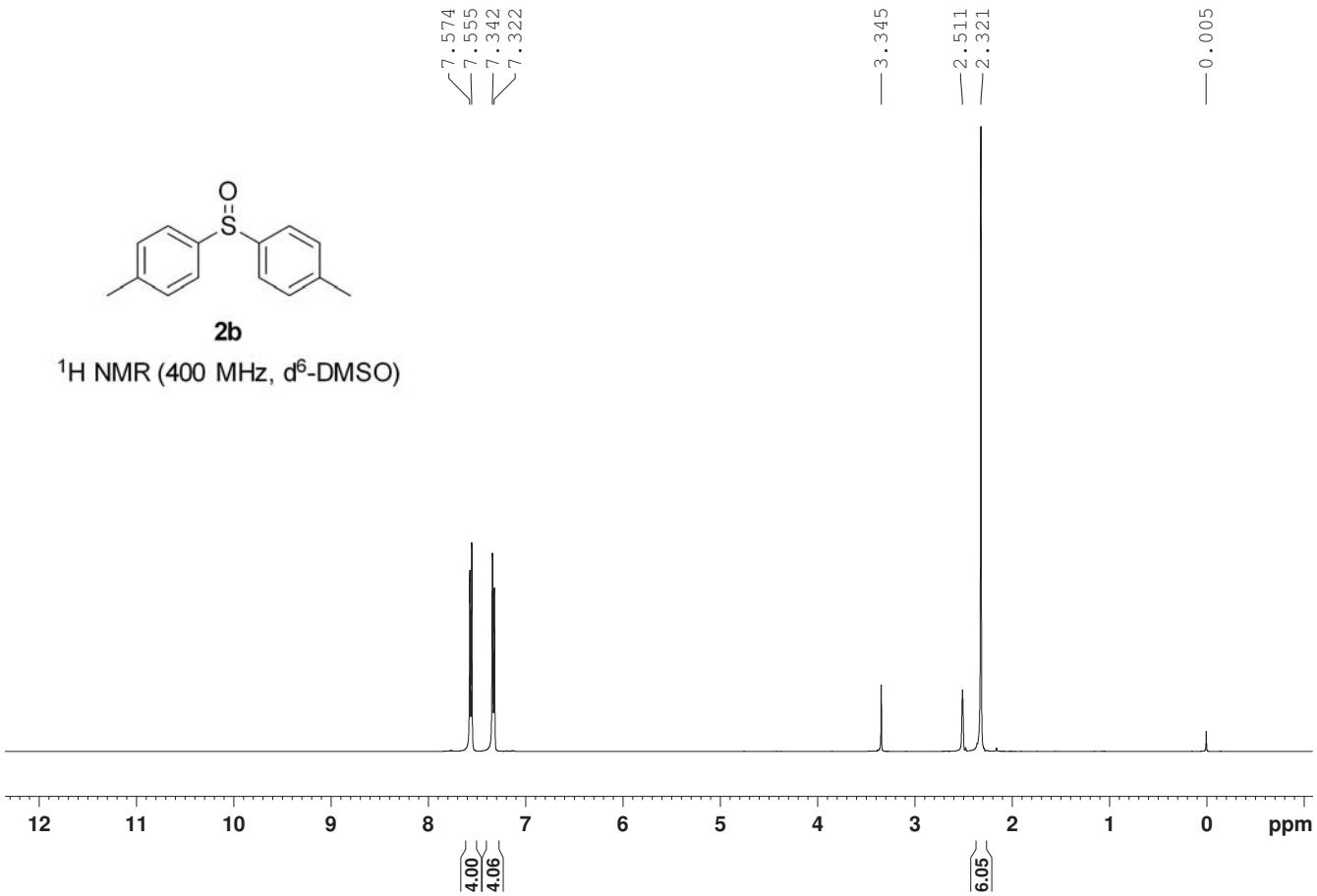
5. NMR Spectra

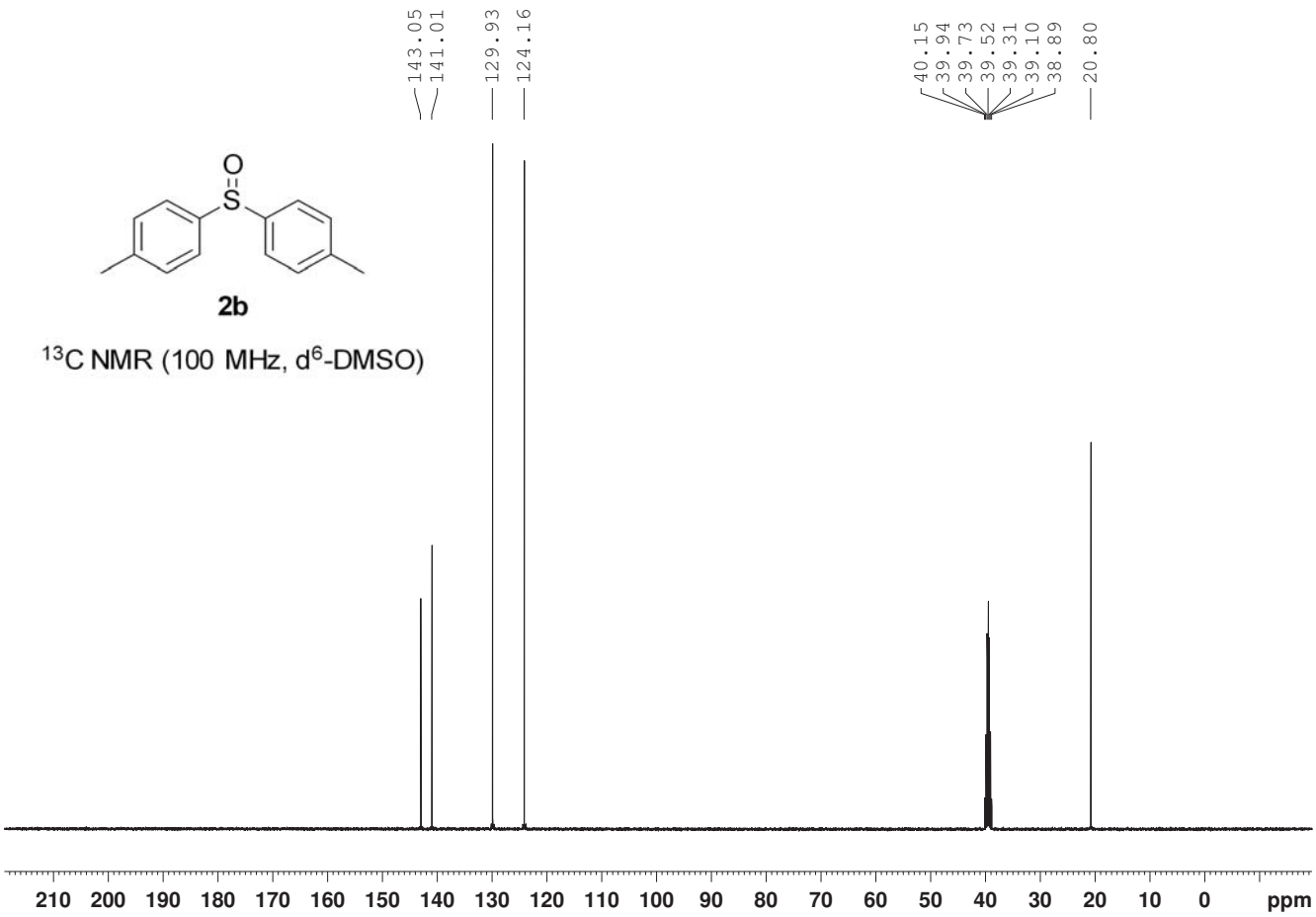






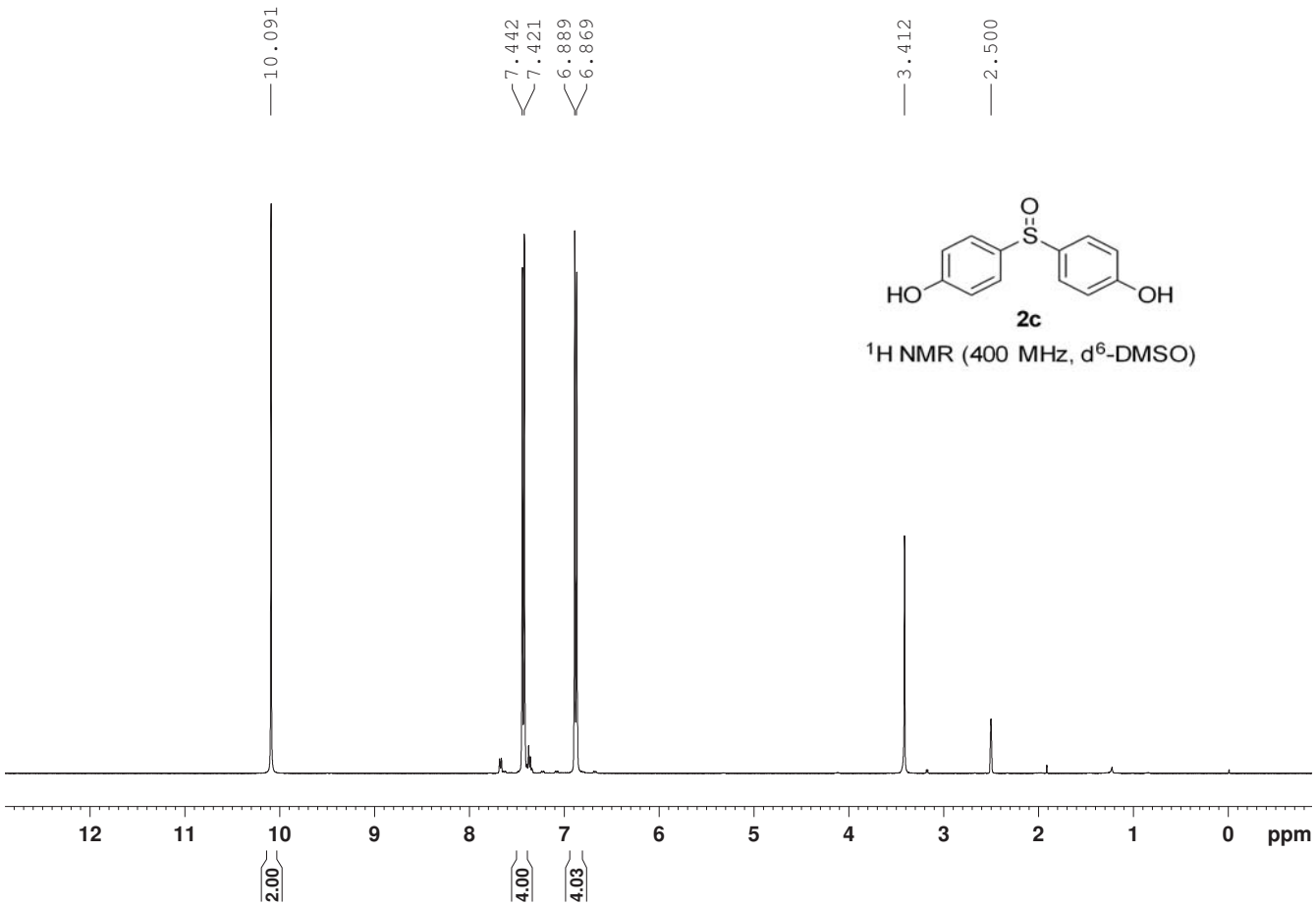
2b

^{1}H NMR (400 MHz, d^{6}-DMSO)



2b

^{13}C NMR (100 MHz, d^{6}-DMSO)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7.421
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HO
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1H NMR (400 MHz, d6-DMSO)
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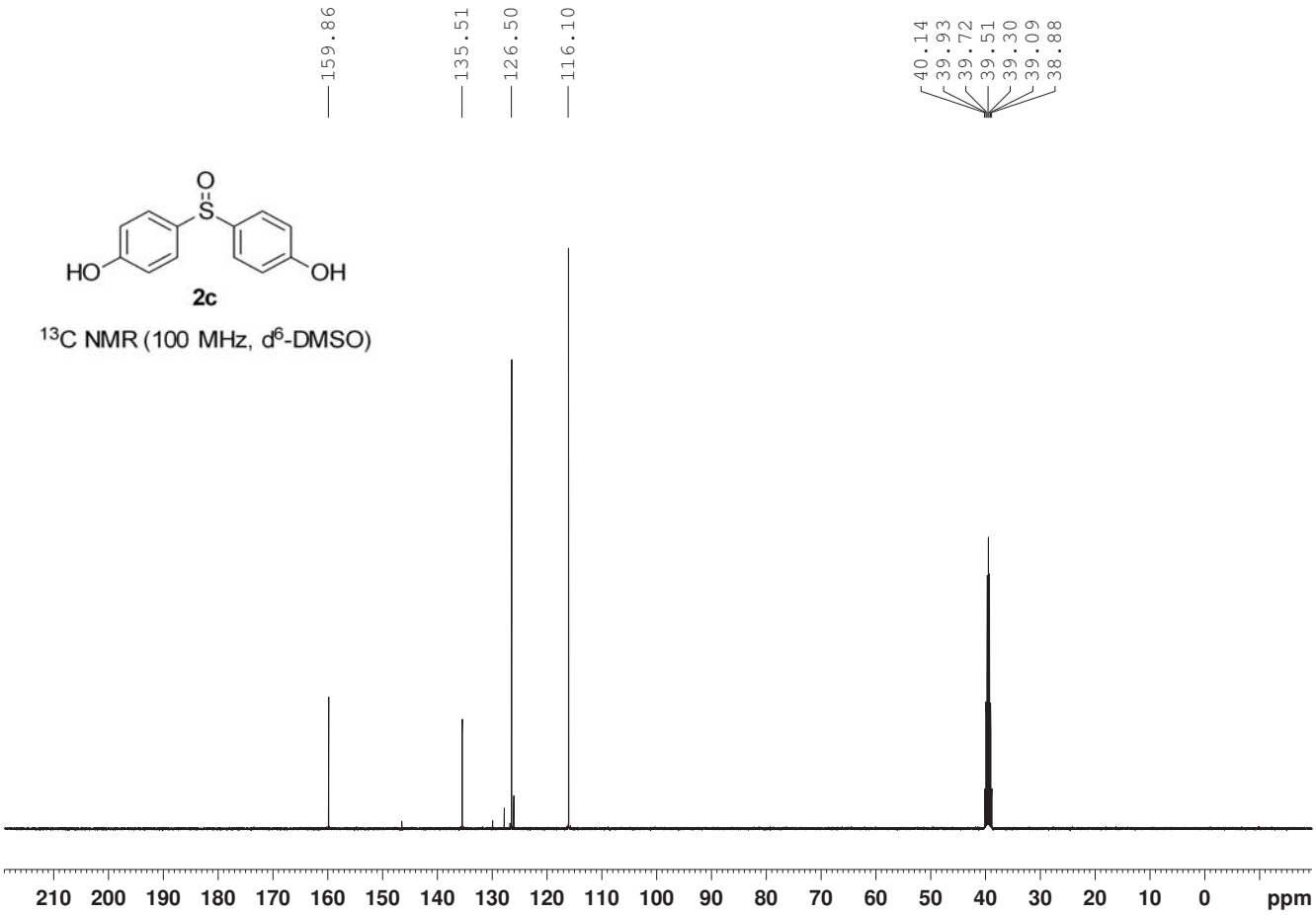
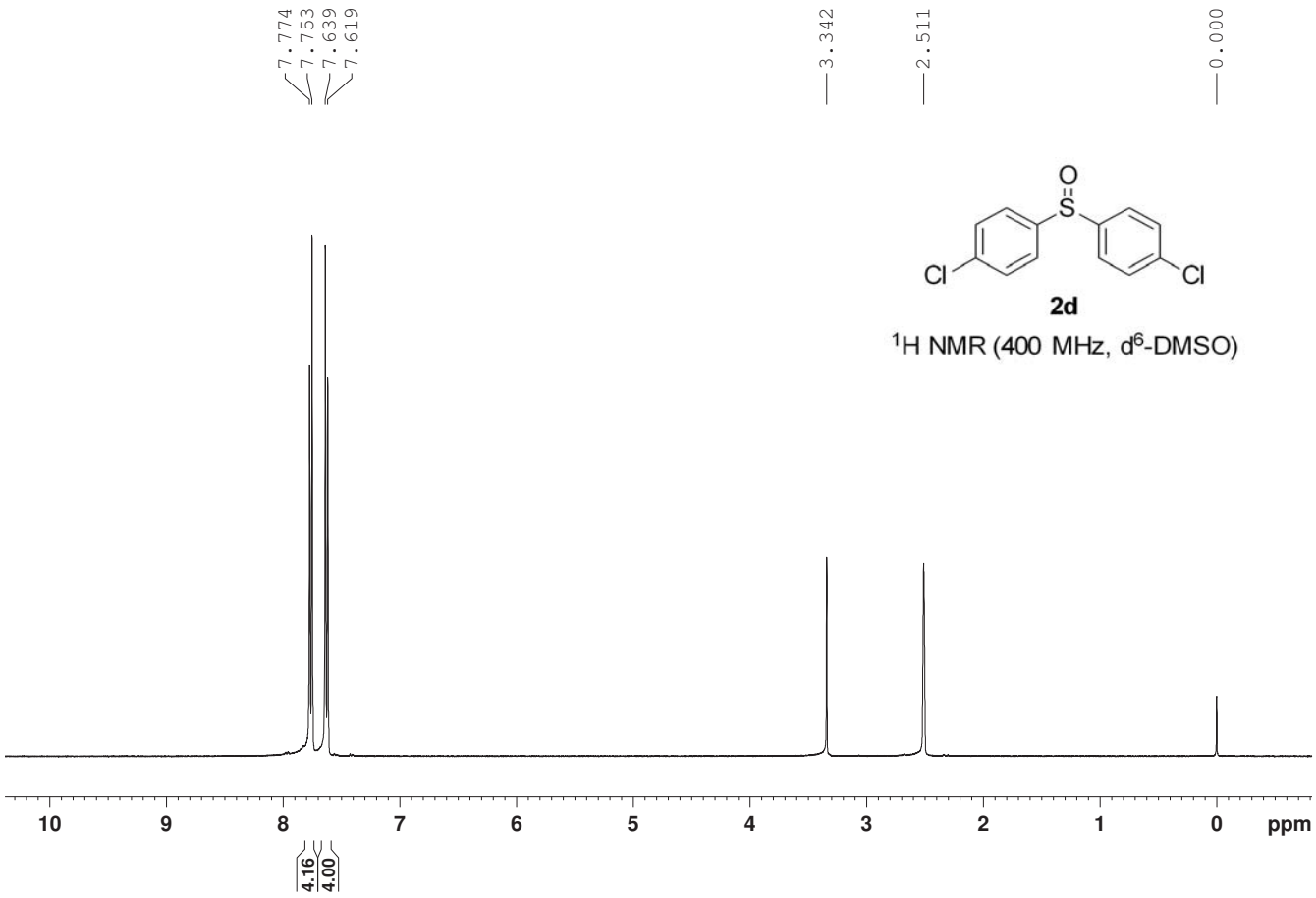
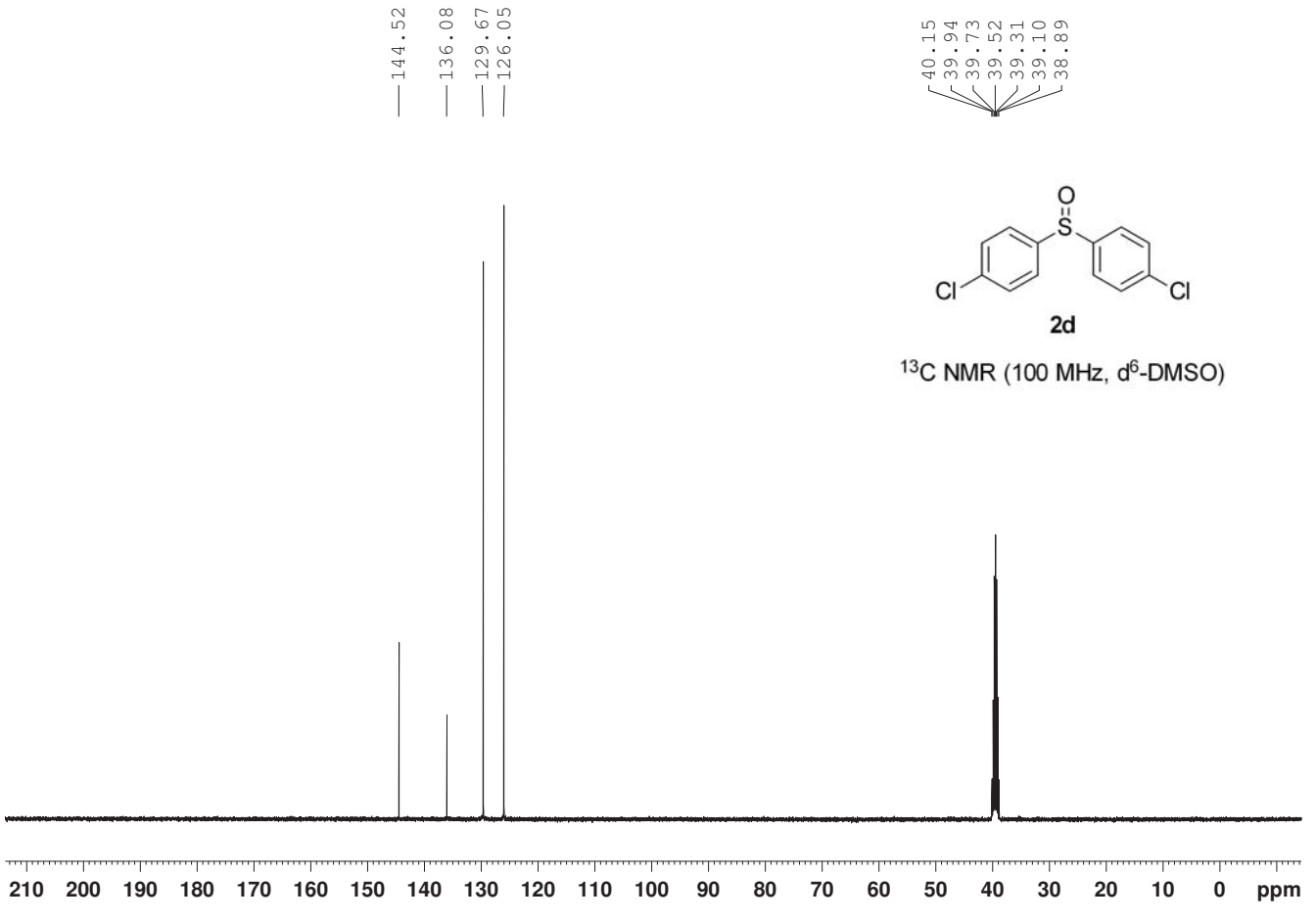
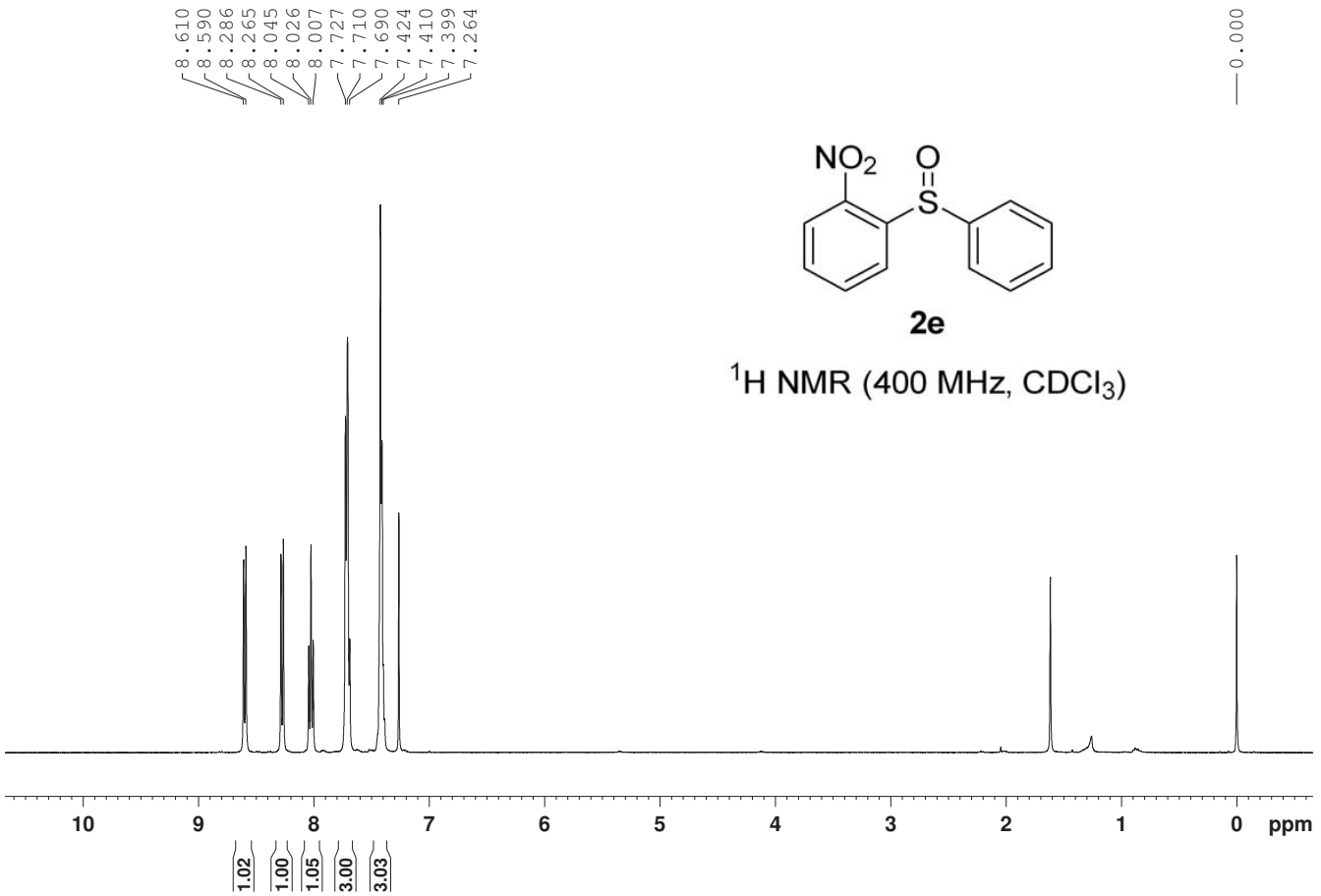
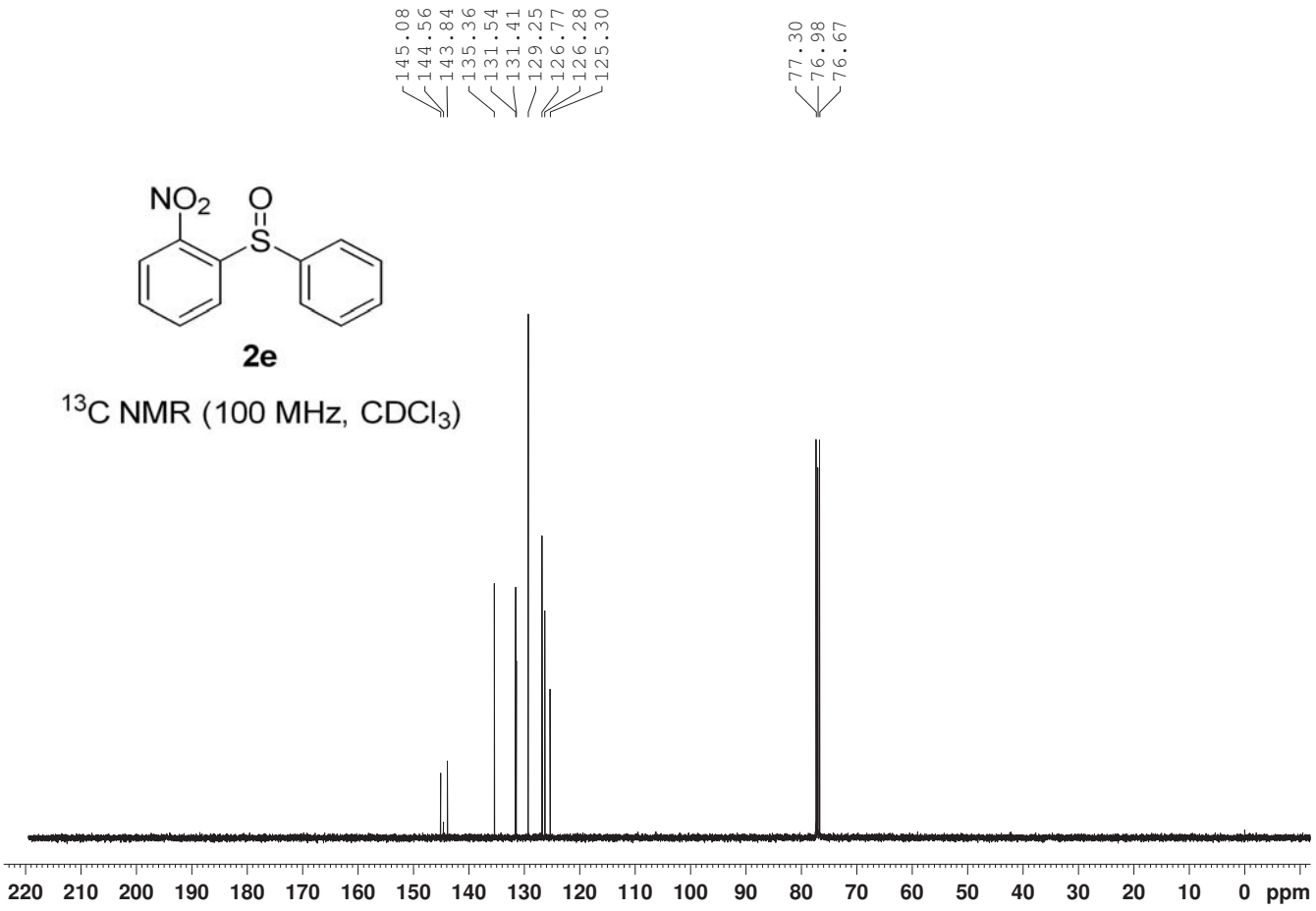
2.00
4.00
4.03

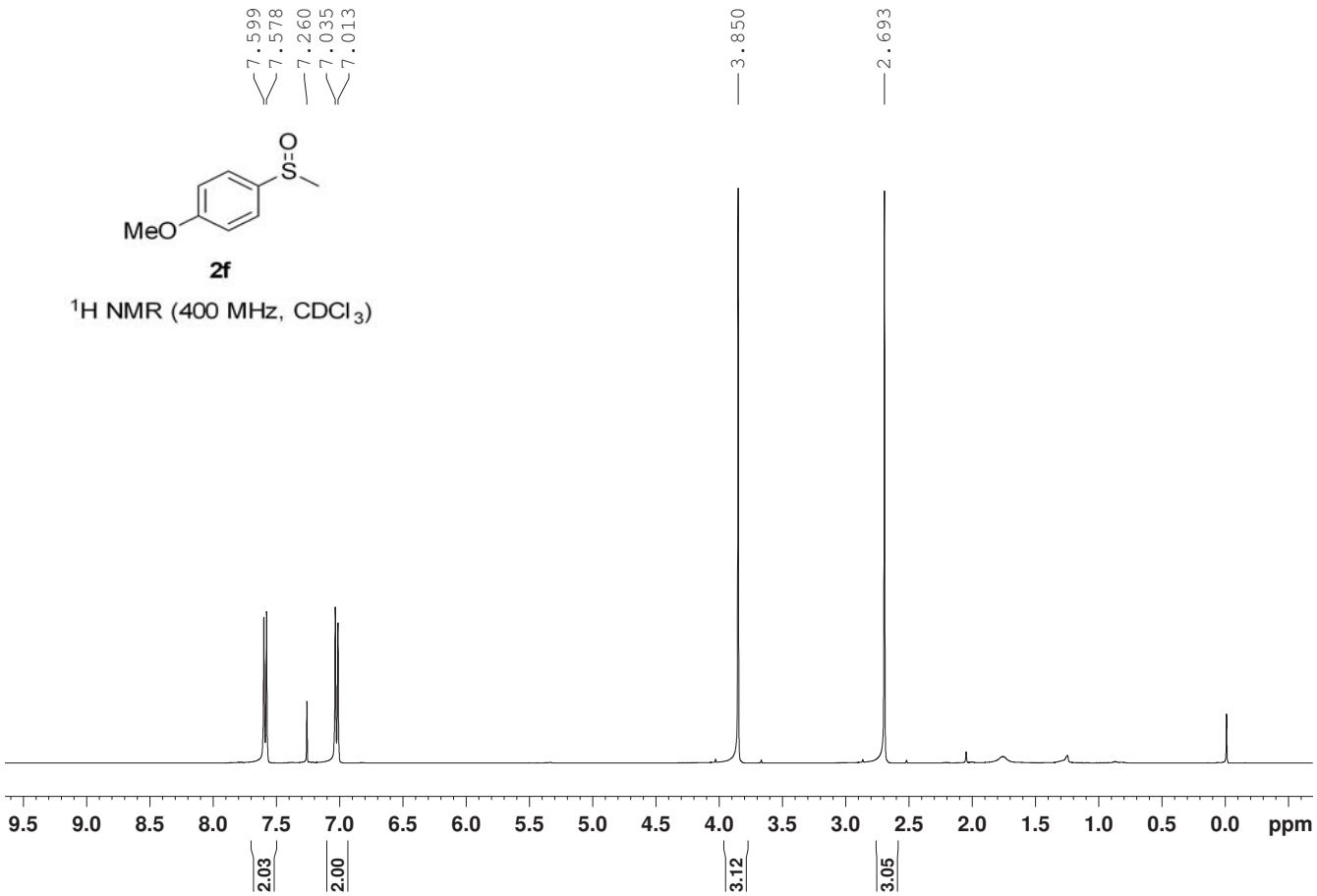

159.86
135.51
126.50
116.10
40.14
39.93
39.72
39.51
39.30
39.09
38.88
HO
OH
2c
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.774
7.753
7.639
7.619
3.342
2.511
0.000
O
S
Cl
Cl
2d
1H NMR (400 MHz, d6-DMSO)
10
9
8
7
6
5
4
3
2
1
0
ppm
4.16
4.00


144.52
136.08
129.67
126.05
40.15
39.94
39.73
39.52
39.31
39.10
38.89
O
S
Cl
Cl
2d
13C NMR (100 MHz, d6-DMSO)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

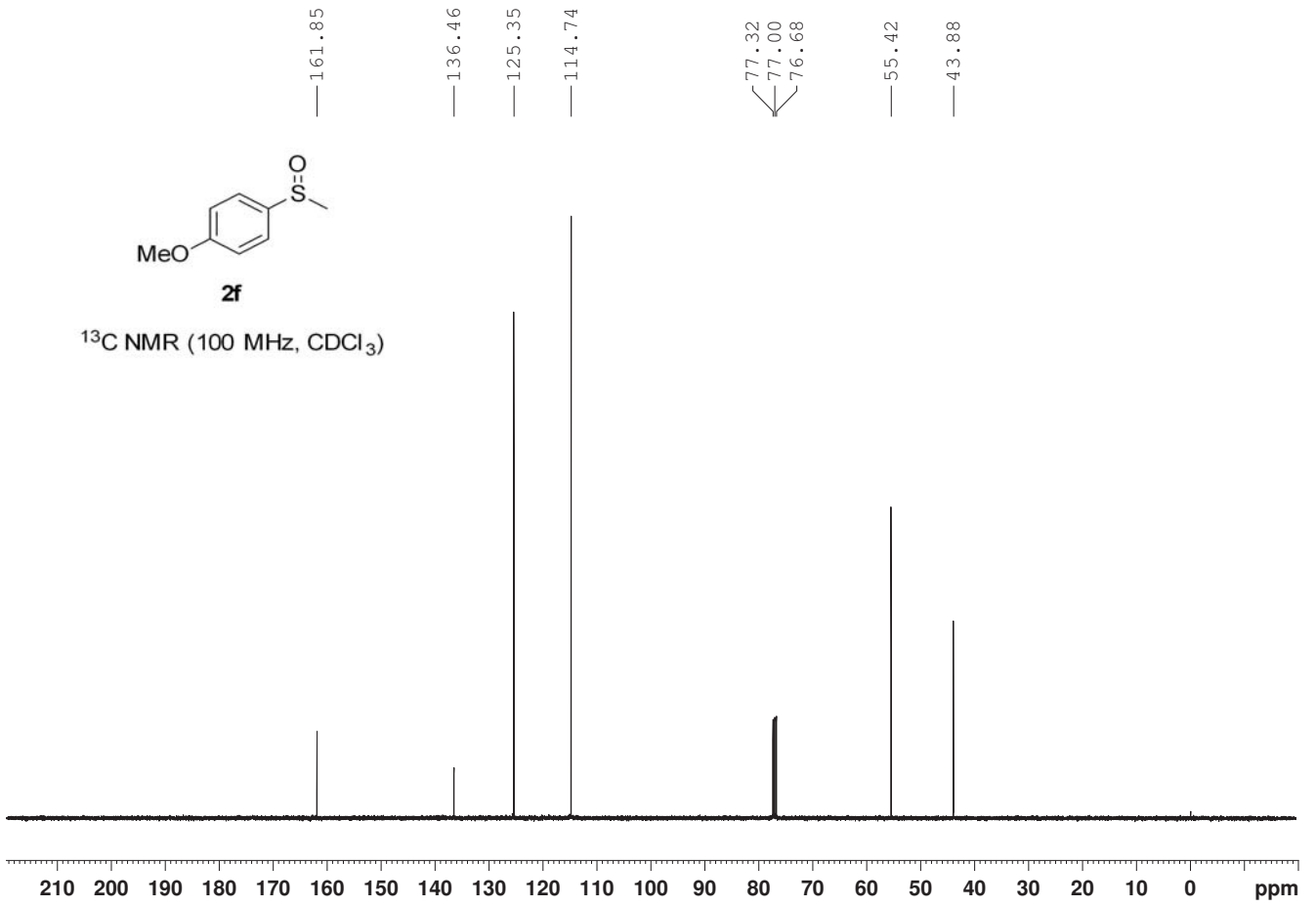

8.610
8.590
8.286
8.265
8.045
8.026
8.007
7.727
7.710
7.690
7.424
7.410
7.399
7.264
0.000
NO2
O
S
2e
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.00
1.05
3.00
3.03


145.08
144.56
143.84
135.36
131.54
131.41
129.25
126.77
126.28
125.30
77.30
76.98
76.67
NO2
O
S
2e
13C NMR (100 MHz, CDCl3)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



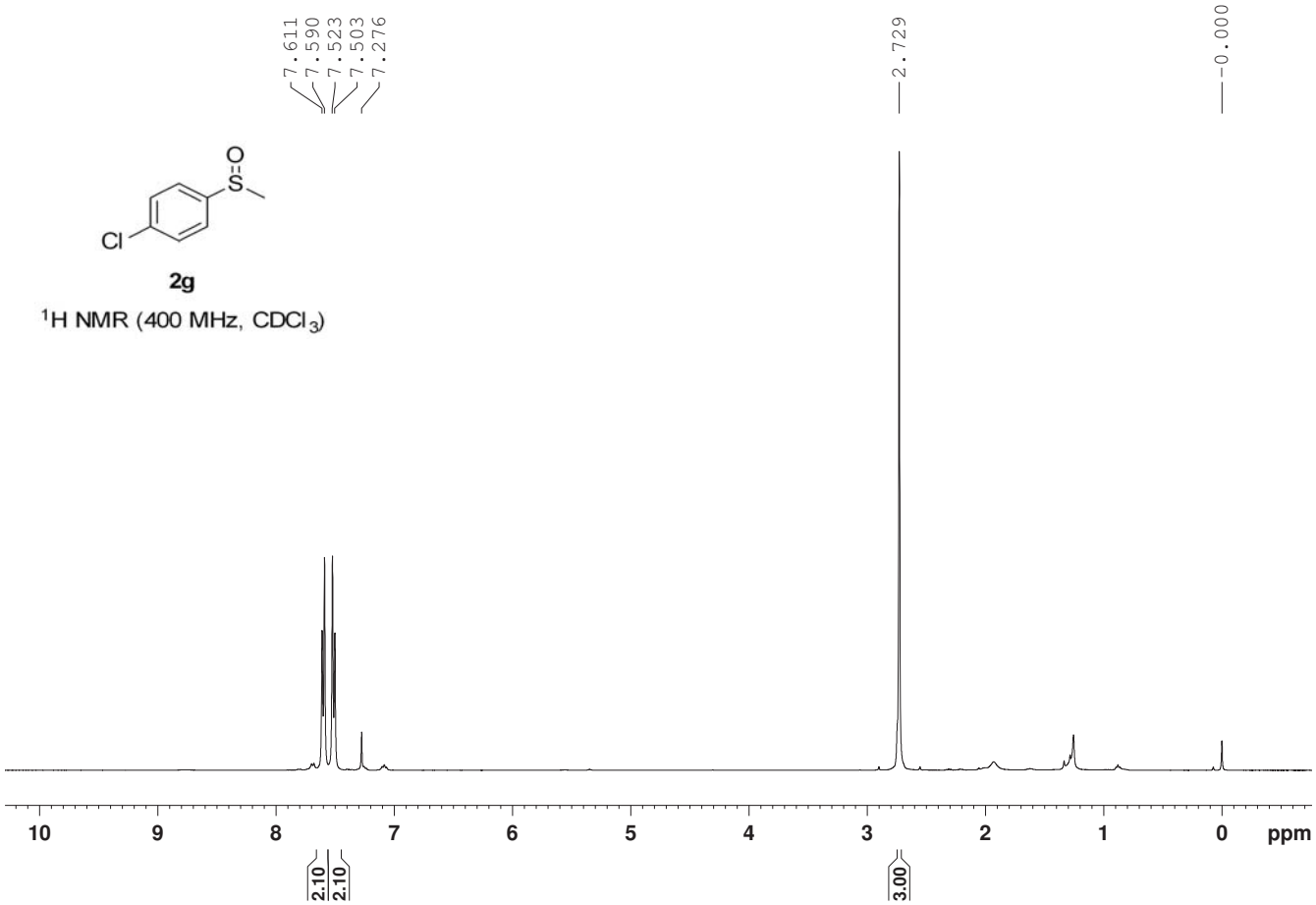
2f

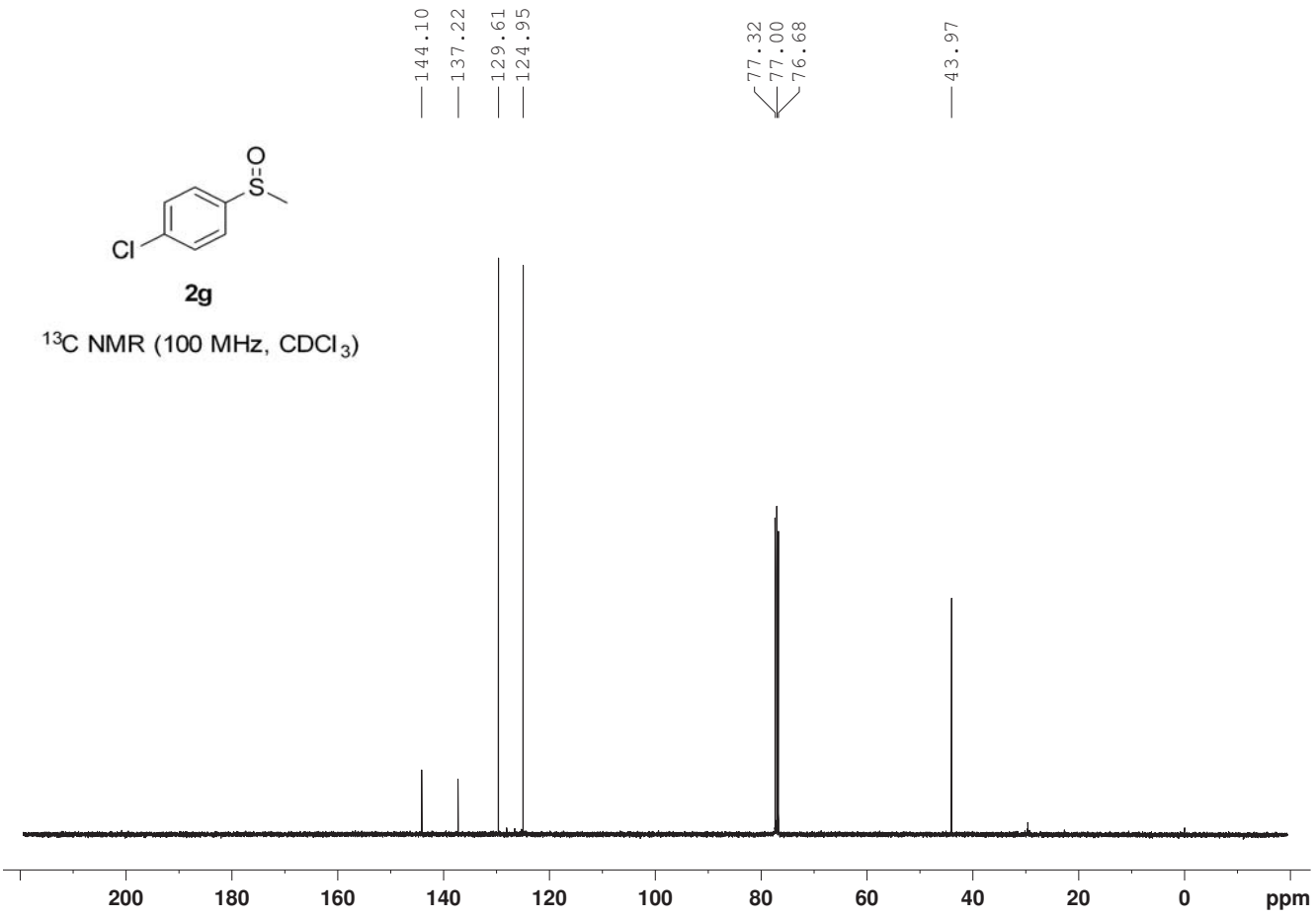
^{1}H NMR (400 MHz, $CDCl_3$)

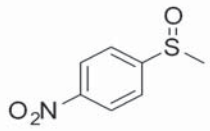


2f

^{13}C NMR (100 MHz, $CDCl_3$)

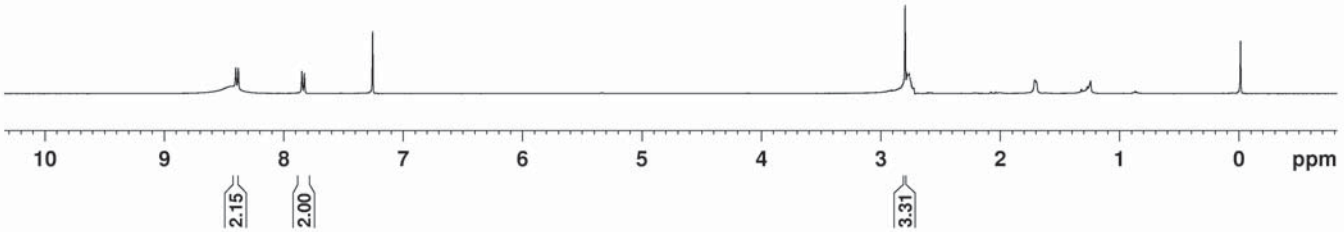

7.611
7.590
7.523
7.503
7.276
2.729
0.000
Cl
O
S
2g
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0
ppm
2.10
2.10
3.00

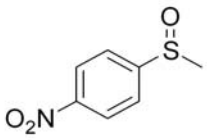

144.10
137.22
129.61
124.95
77.32
77.00
76.68
43.97
Cl
O
S
2g
13C NMR (100 MHz, CDCl3)
200
180
160
140
120
100
80
60
40
20
0
ppm



2h

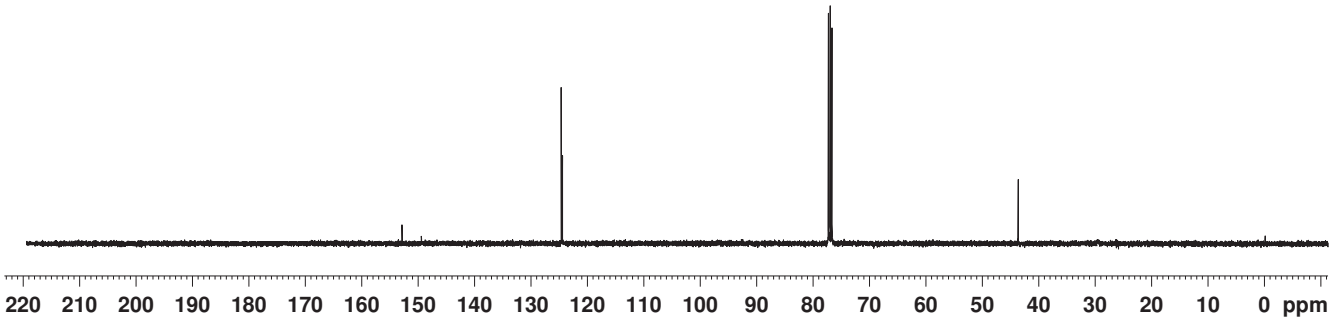
^{1}H NMR (400 MHz, $CDCl_3$)

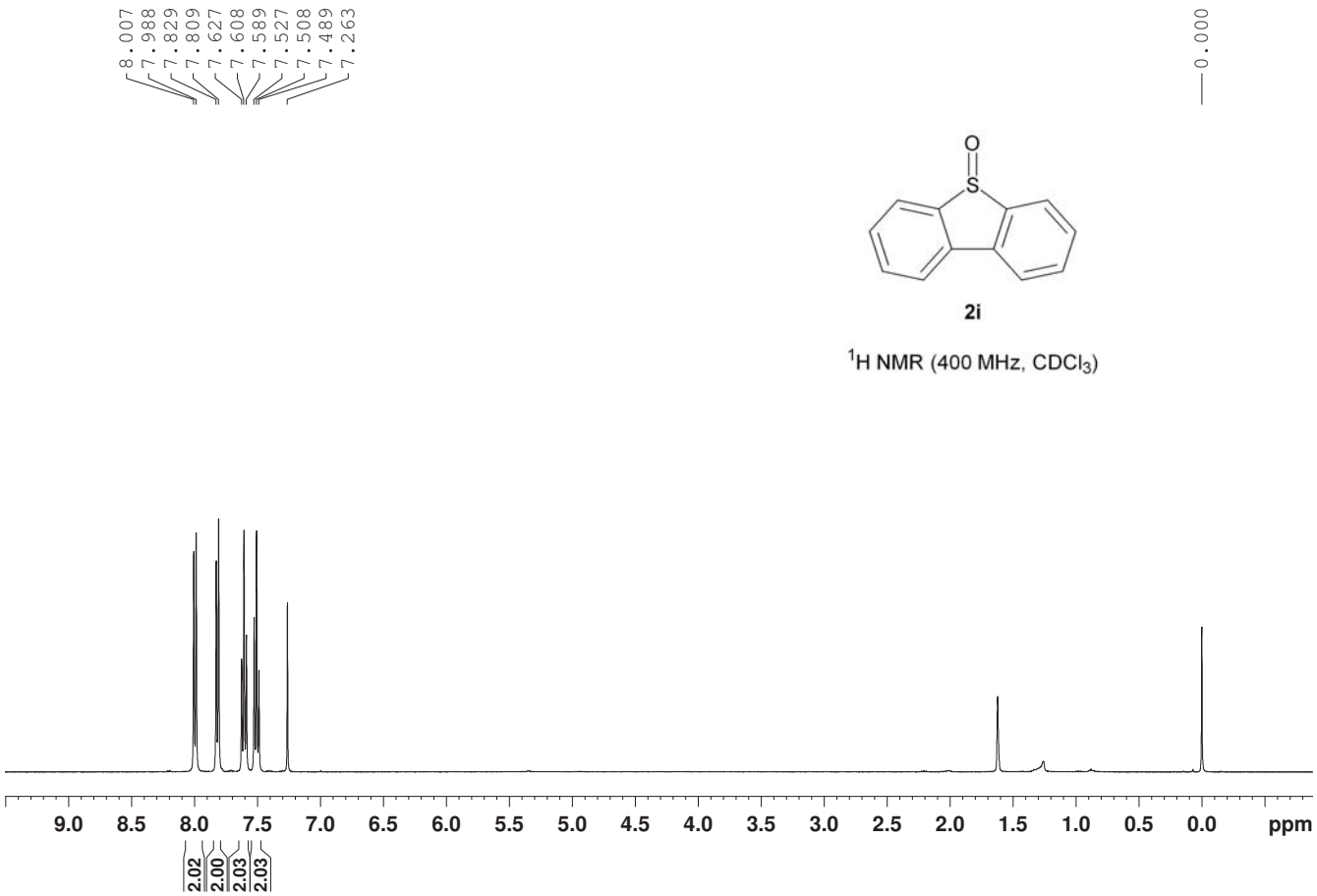


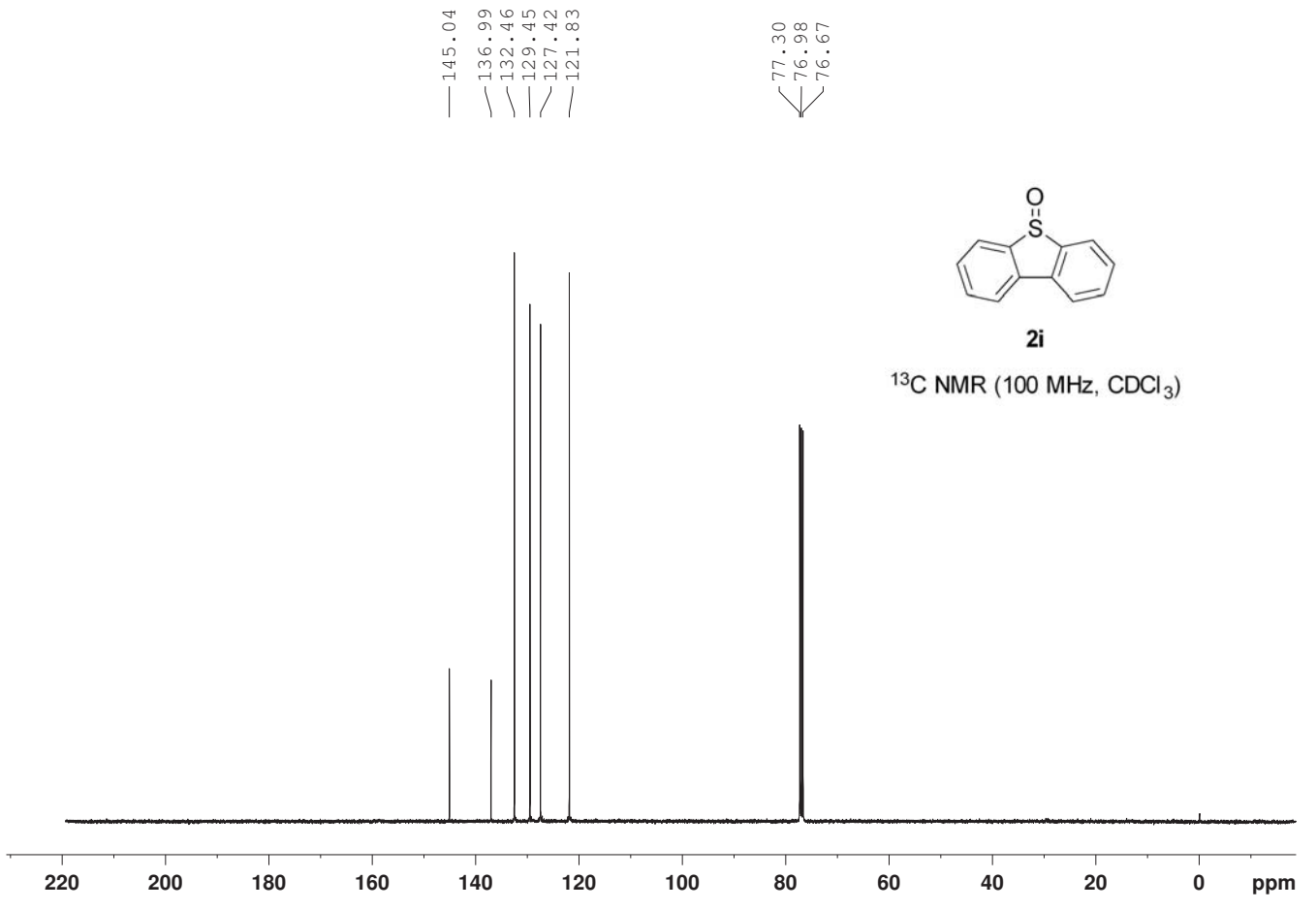


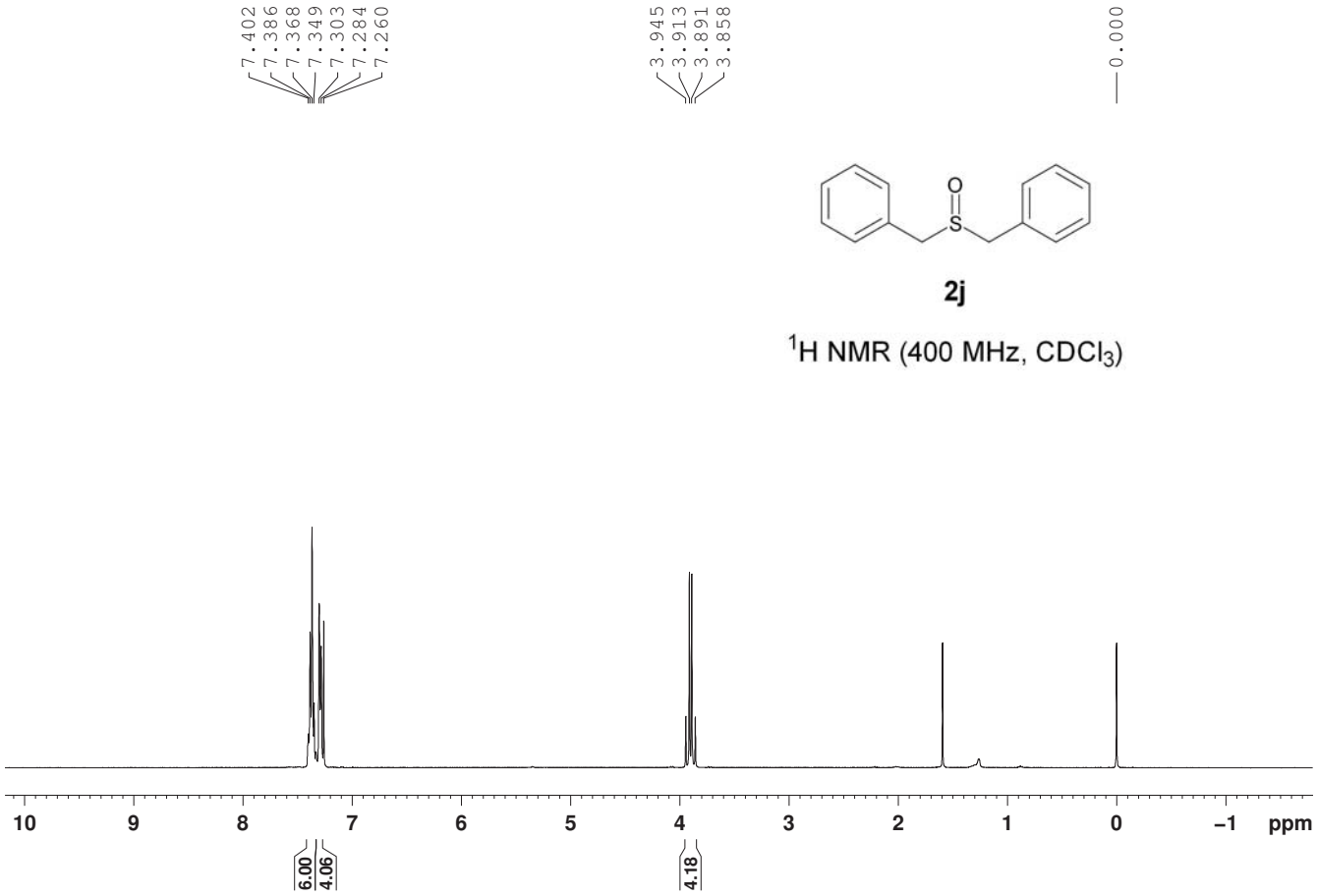
2h

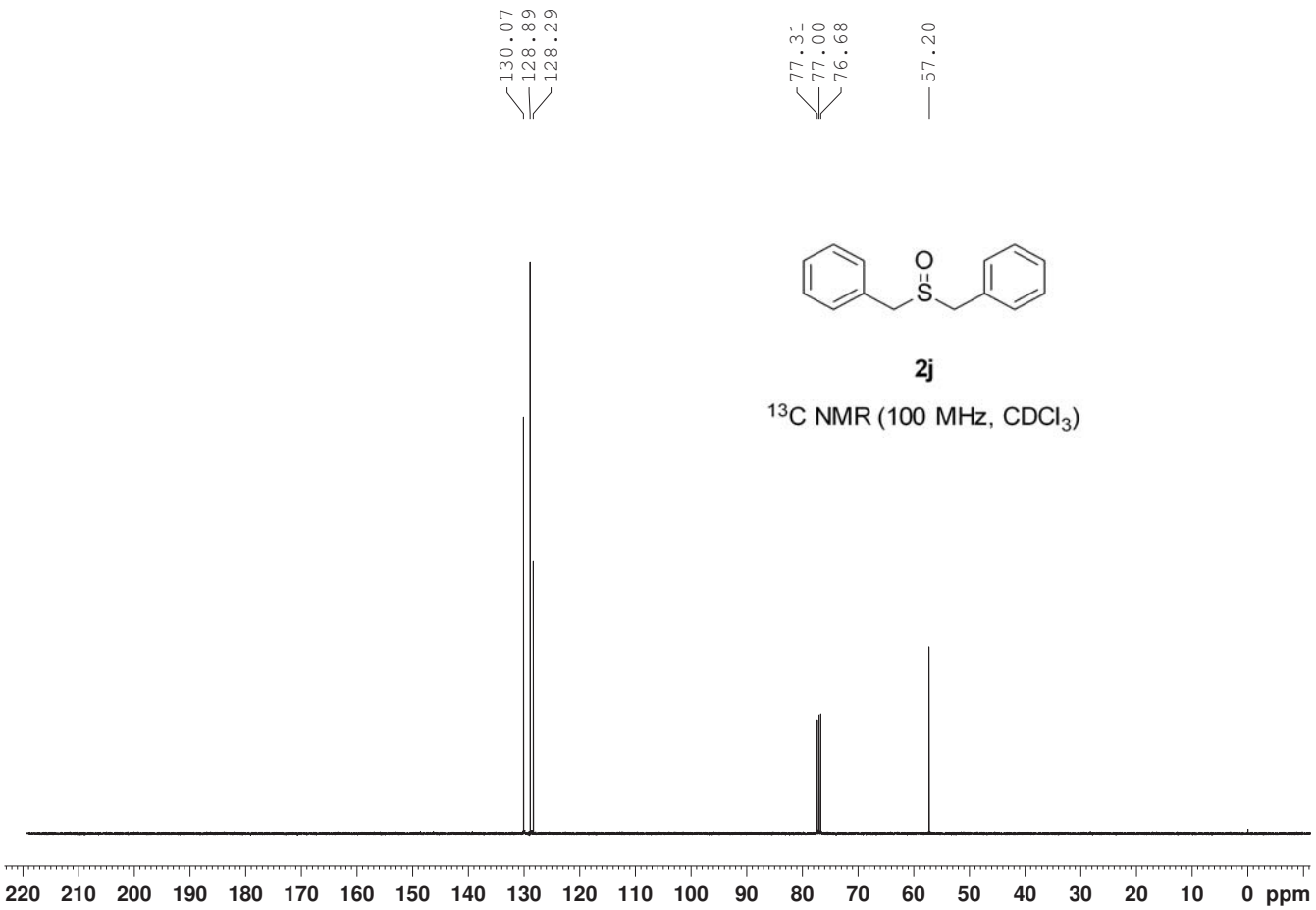
^{13}C NMR (100 MHz, $CDCl_3$)

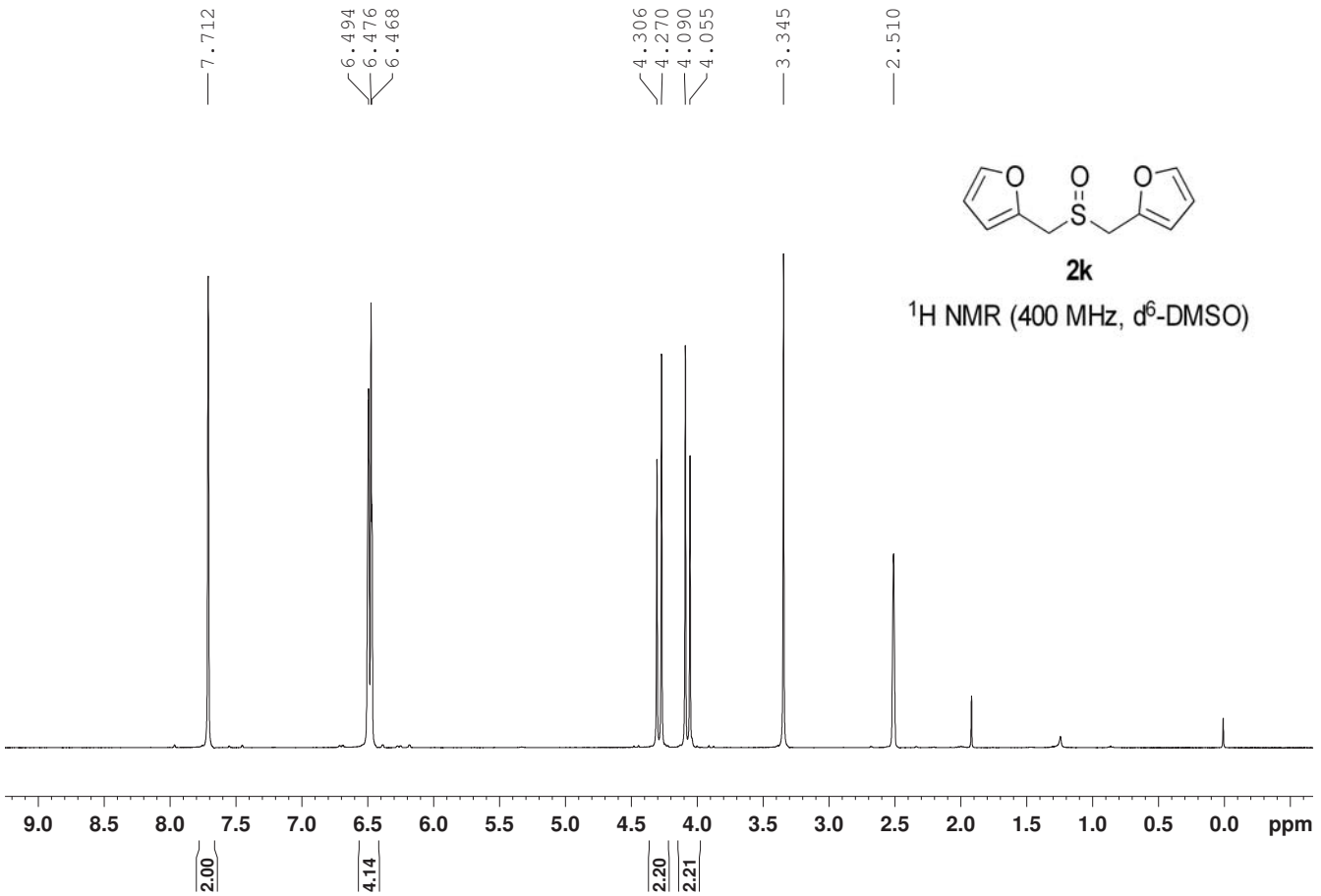


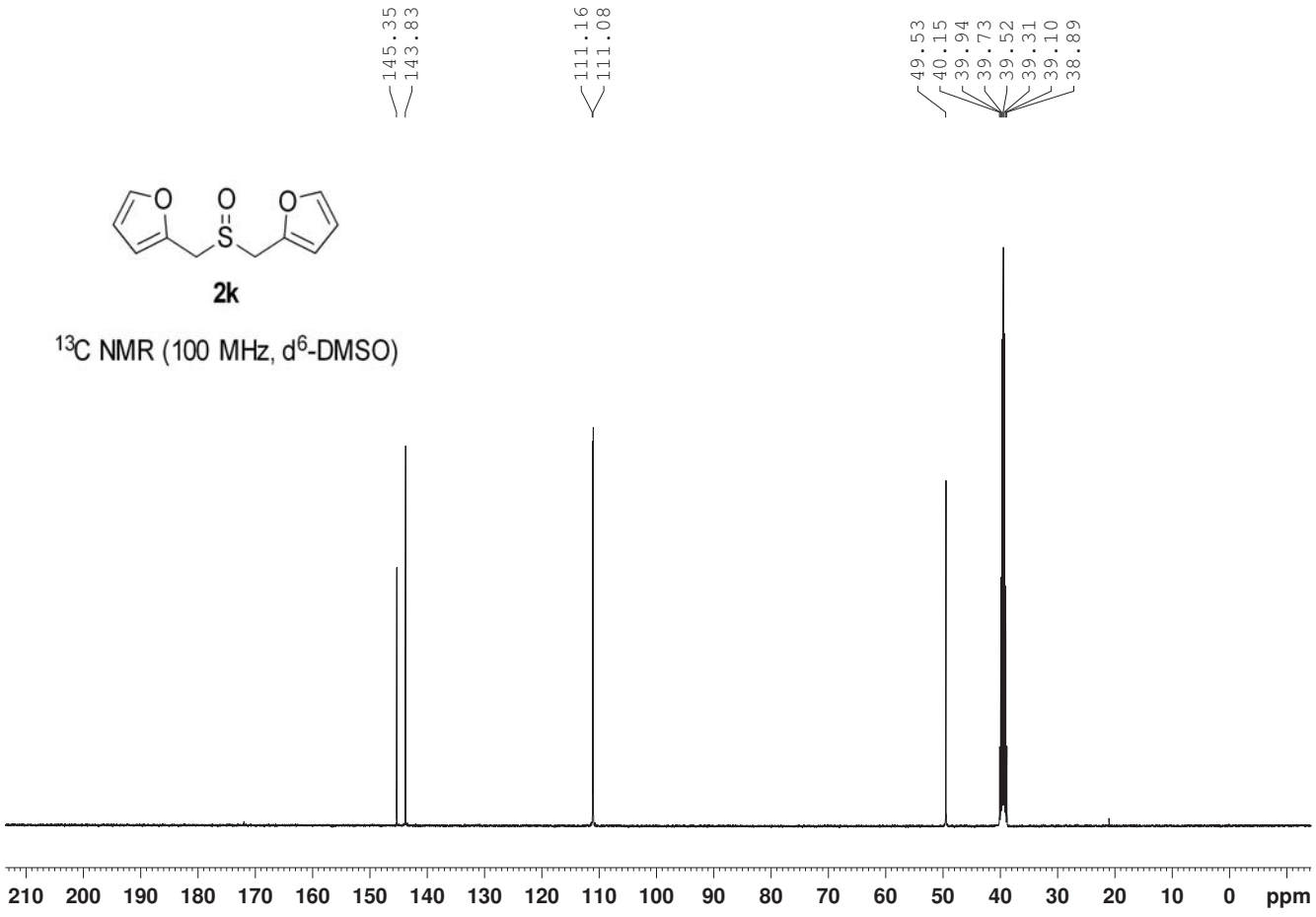

8.007
7.988
7.829
7.809
7.627
7.608
7.589
7.527
7.508
7.489
7.263
0.000
O
S
2i
^{1}H NMR (400 MHz, CDCl$_3$)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.02
2.00
2.03
2.03

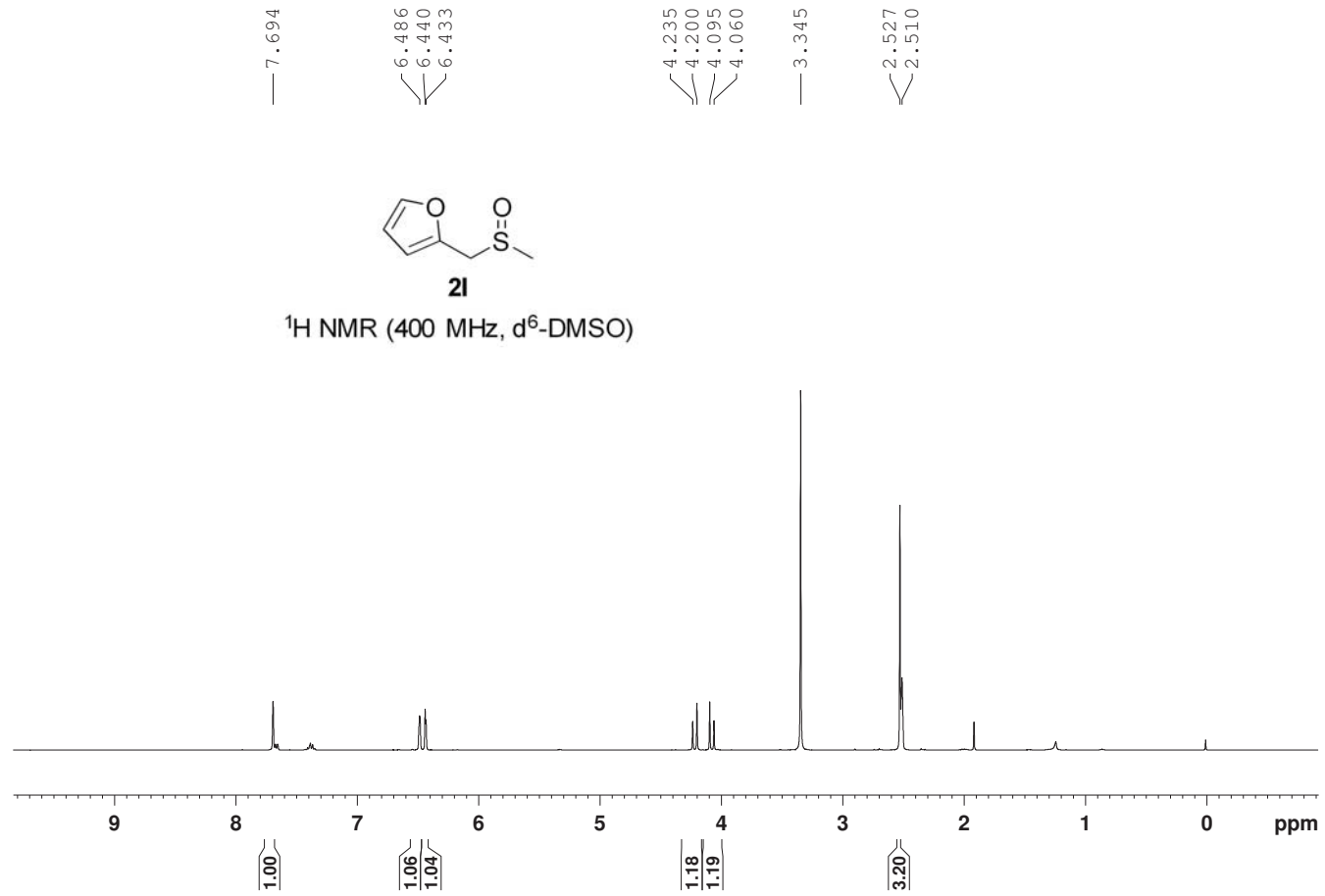

145.04
136.99
132.46
129.45
127.42
121.83
77.30
76.98
76.67
O
S
2i
^{13}C NMR (100 MHz, CDCl$_3$)
220 200 180 160 140 120 100 80 60 40 20 0 ppm

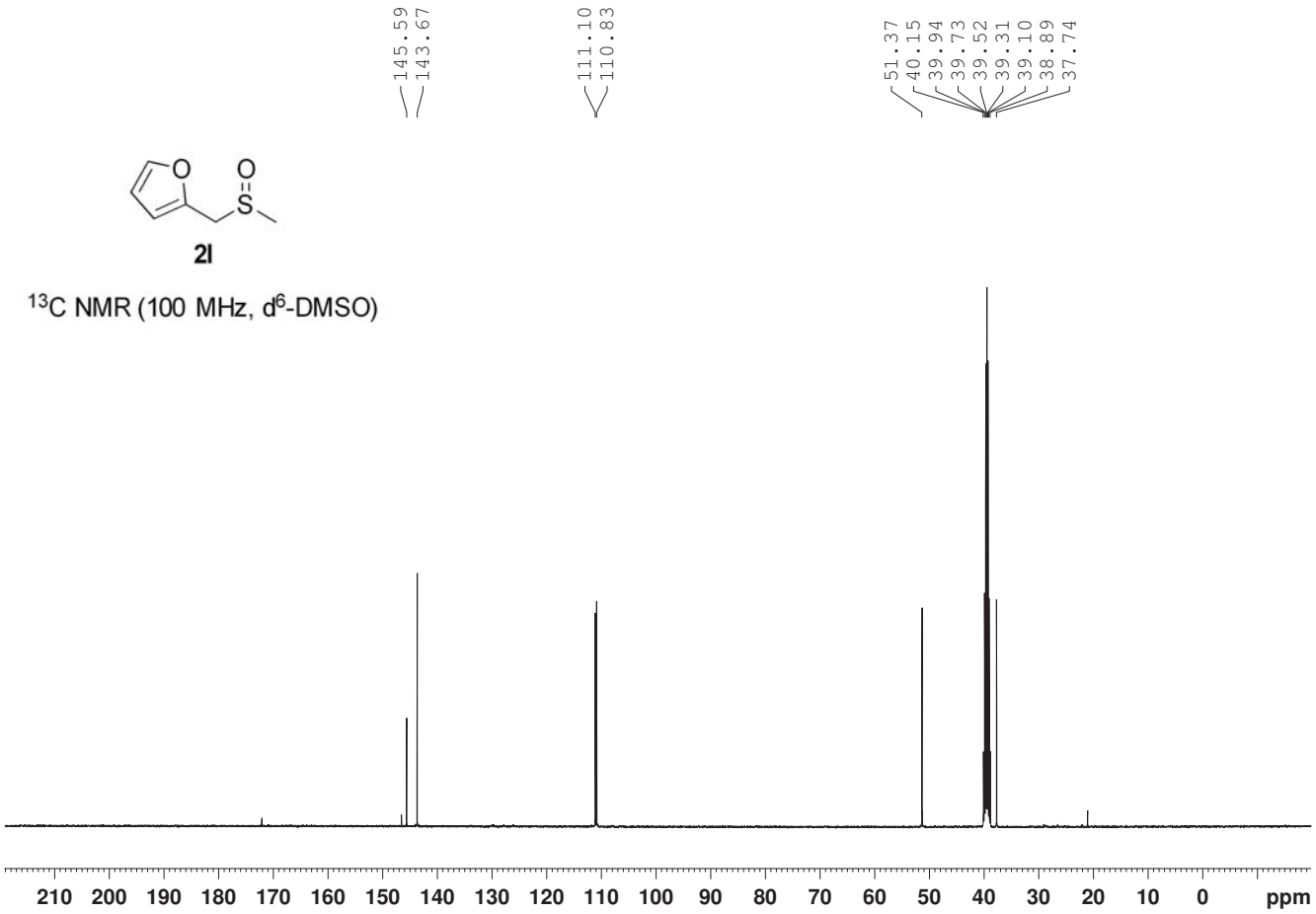

7.402
7.386
7.368
7.349
7.303
7.284
7.260
3.945
3.913
3.891
3.858
0.000
O
S
2j
^{1}H NMR (400 MHz, $CDCl_3$)
10
9
8
7
6
5
4
3
2
1
0
–1
ppm
6.00
4.06
4.18

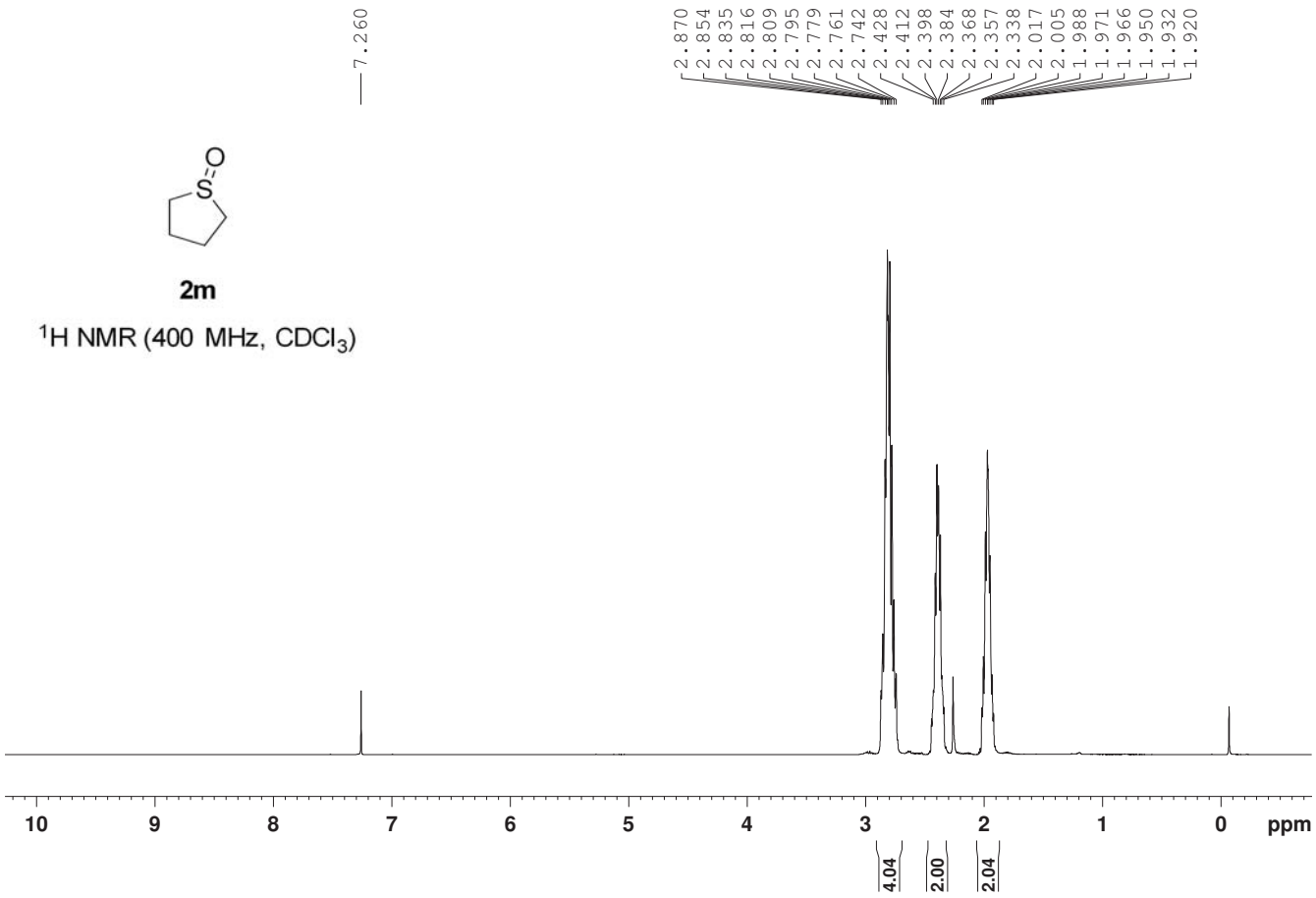

130.07
128.89
128.29
77.31
77.00
76.68
57.20
O
S
2j
^{13}C NMR (100 MHz, $CDCl_3$)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

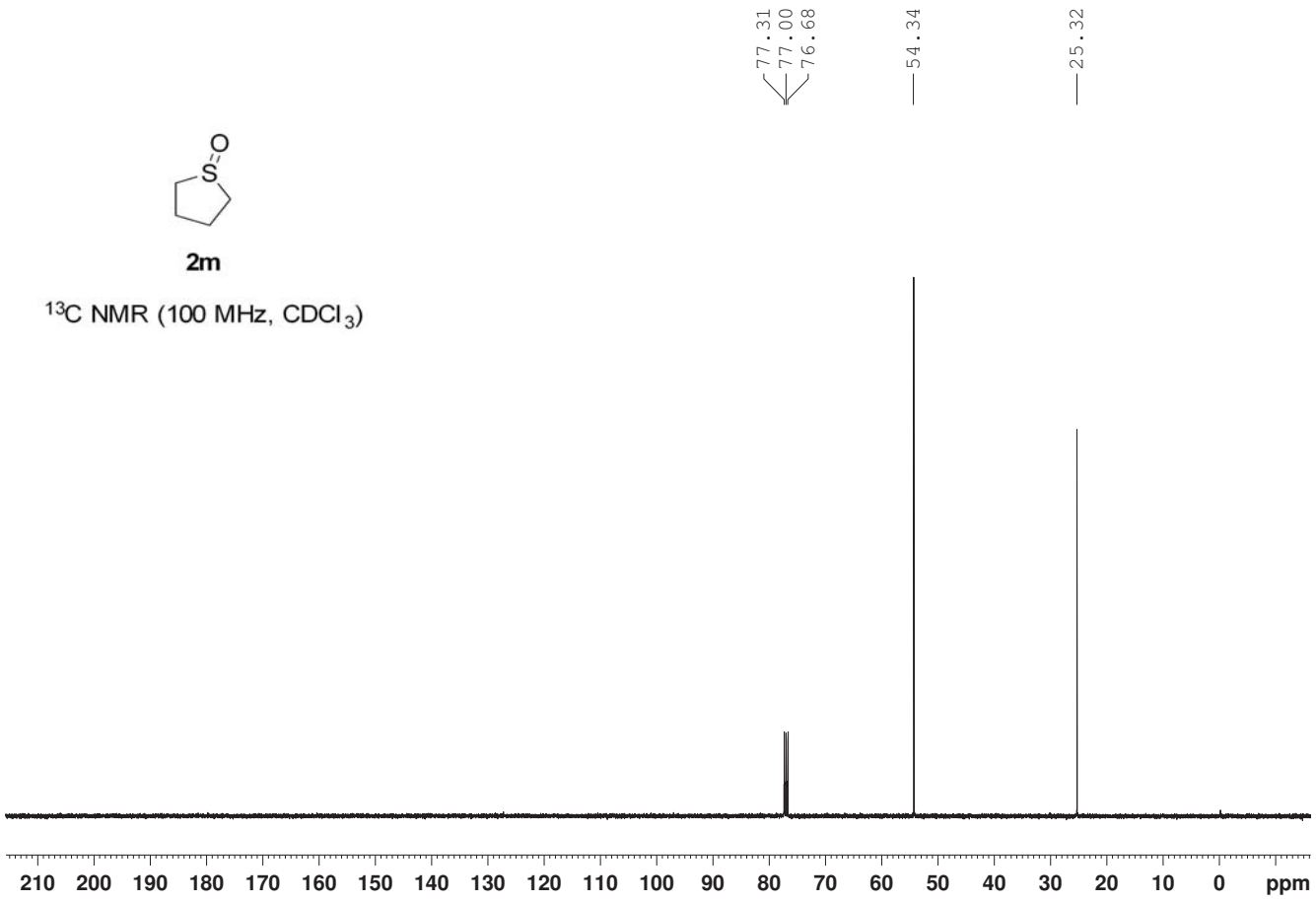

7.712
6.494
6.476
6.468
4.306
4.270
4.090
4.055
3.345
2.510
2k
1H NMR (400 MHz, d6-DMSO)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
4.14
2.20
2.21

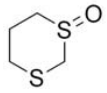

145.35
143.83
111.16
111.08
49.53
40.15
39.94
39.73
39.52
39.31
39.10
38.89
2k
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.694
6.486
6.440
6.433
4.235
4.200
4.095
4.060
3.345
2.527
2.510
2l
1H NMR (400 MHz, d6-DMSO)
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.06
1.04
1.18
1.19
3.20


145.59
143.67
111.10
110.83
51.37
40.15
39.94
39.73
39.52
39.31
39.10
38.89
37.74
2l
13C NMR (100 MHz, d6-DMSO)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

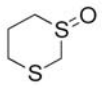

7.260
2.870
2.854
2.835
2.816
2.809
2.795
2.779
2.761
2.742
2.428
2.412
2.398
2.384
2.368
2.357
2.338
2.017
2.005
1.988
1.971
1.966
1.950
1.932
1.920
O
S
2m
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0
ppm
4.04
2.00
2.04


77.31
77.00
76.68
54.34
25.32
O
S
2m
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



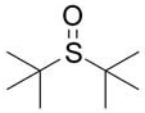
2n

^{1}H NMR (400 MHz, $CDCl_3$)



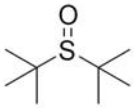
2n

^{13}C NMR (100 MHz, $CDCl_3$)



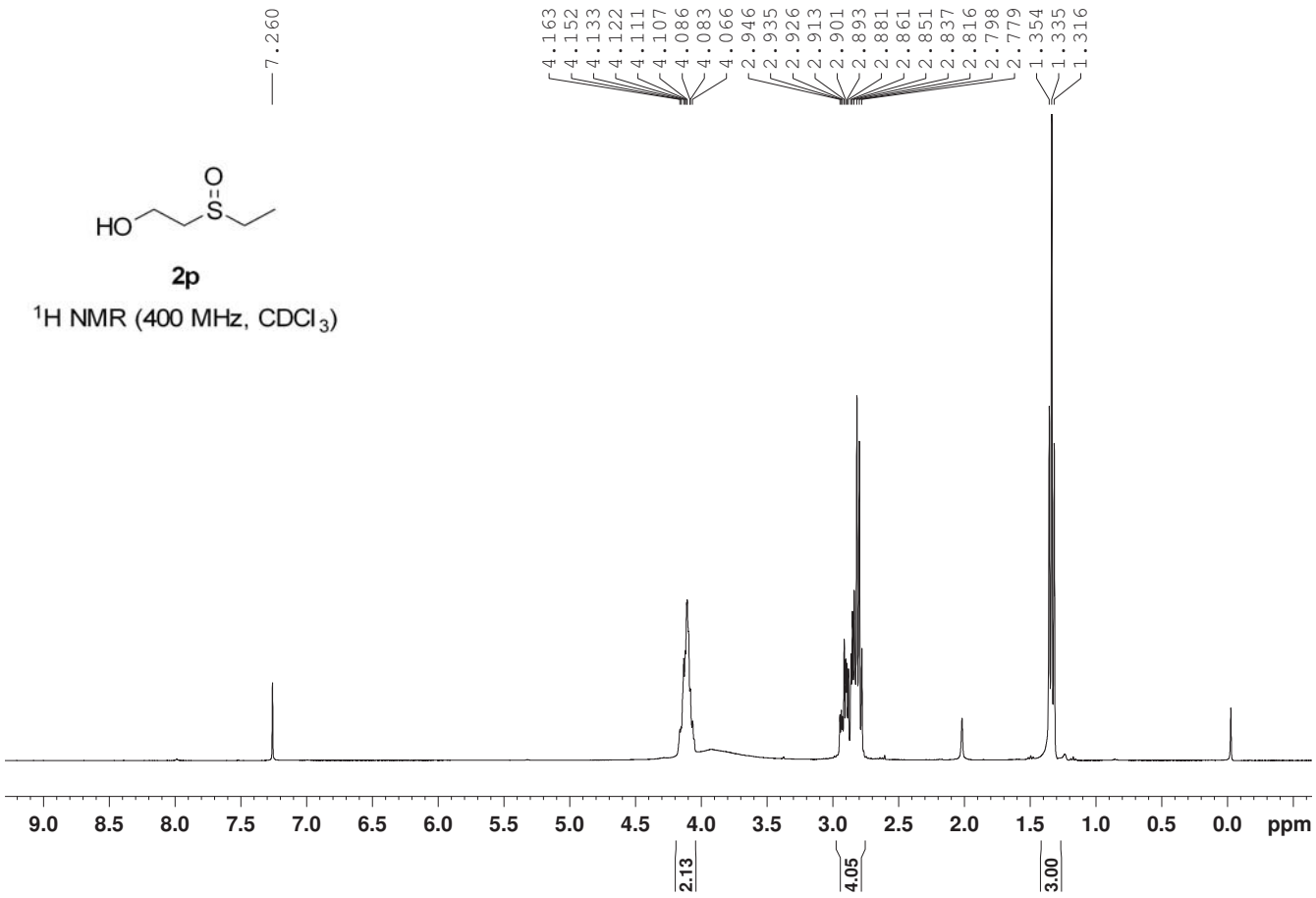
2o

^{1}H NMR (400 MHz, d^{6}-DMSO)



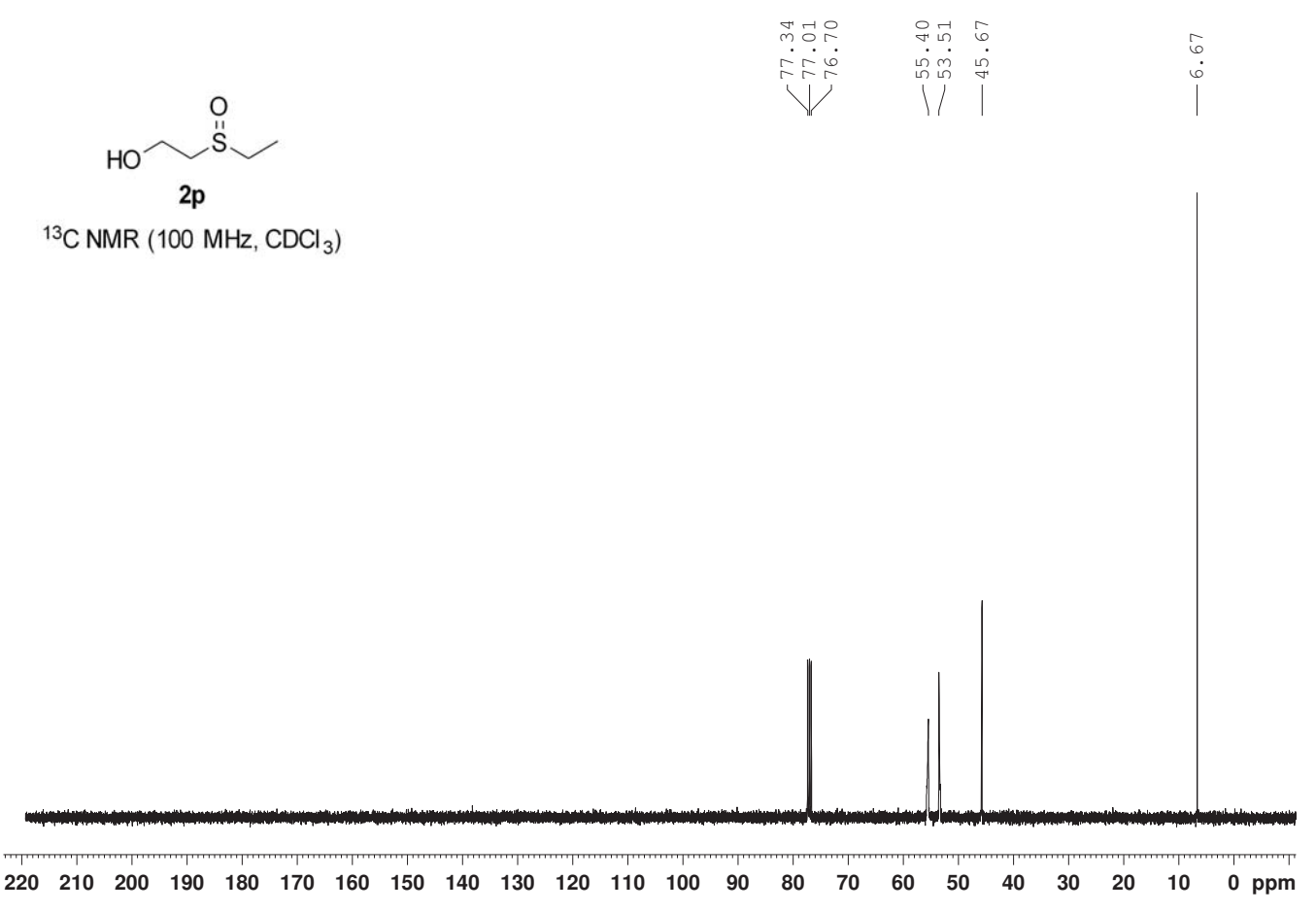
2o

^{13}C NMR (100 MHz, d^{6}-DMSO)



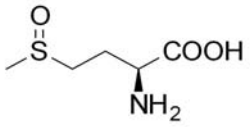
2p

^{1}H NMR (400 MHz, $CDCl_3$)



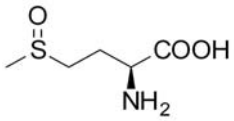
2p

^{13}C NMR (100 MHz, $CDCl_3$)



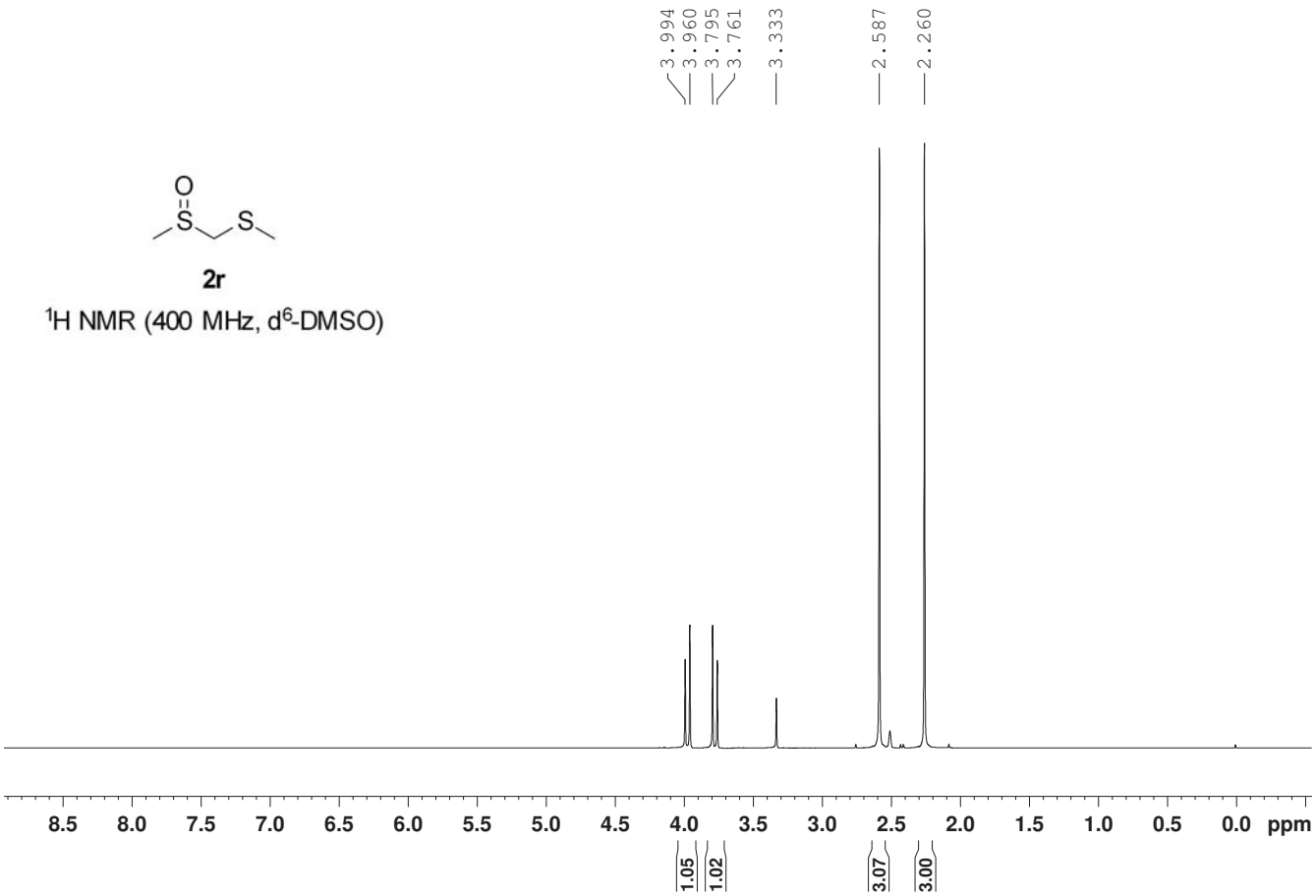
2q

^{1}H NMR (400 MHz, D_2O)



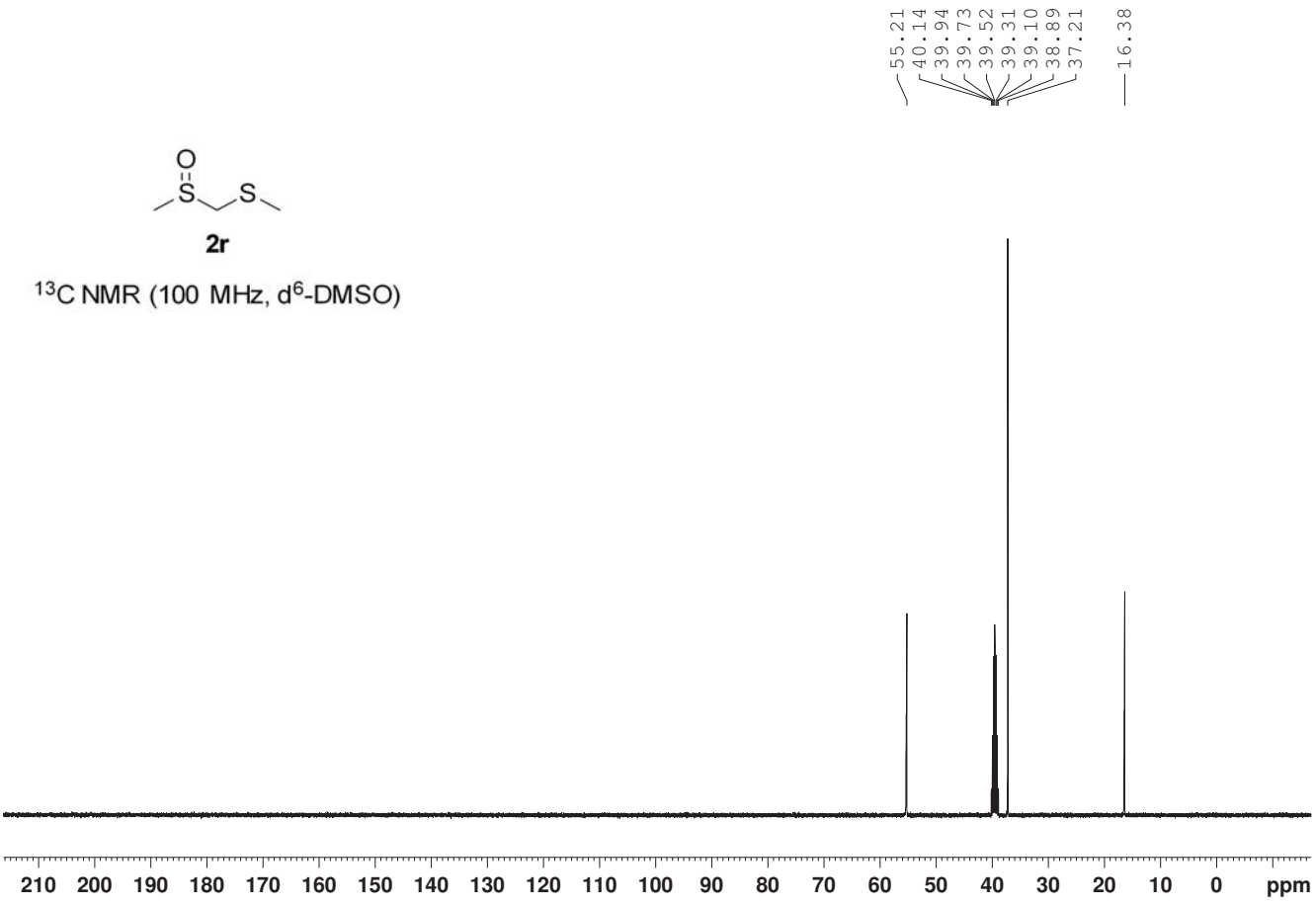
2q

^{13}C NMR (100 MHz, D_2O)



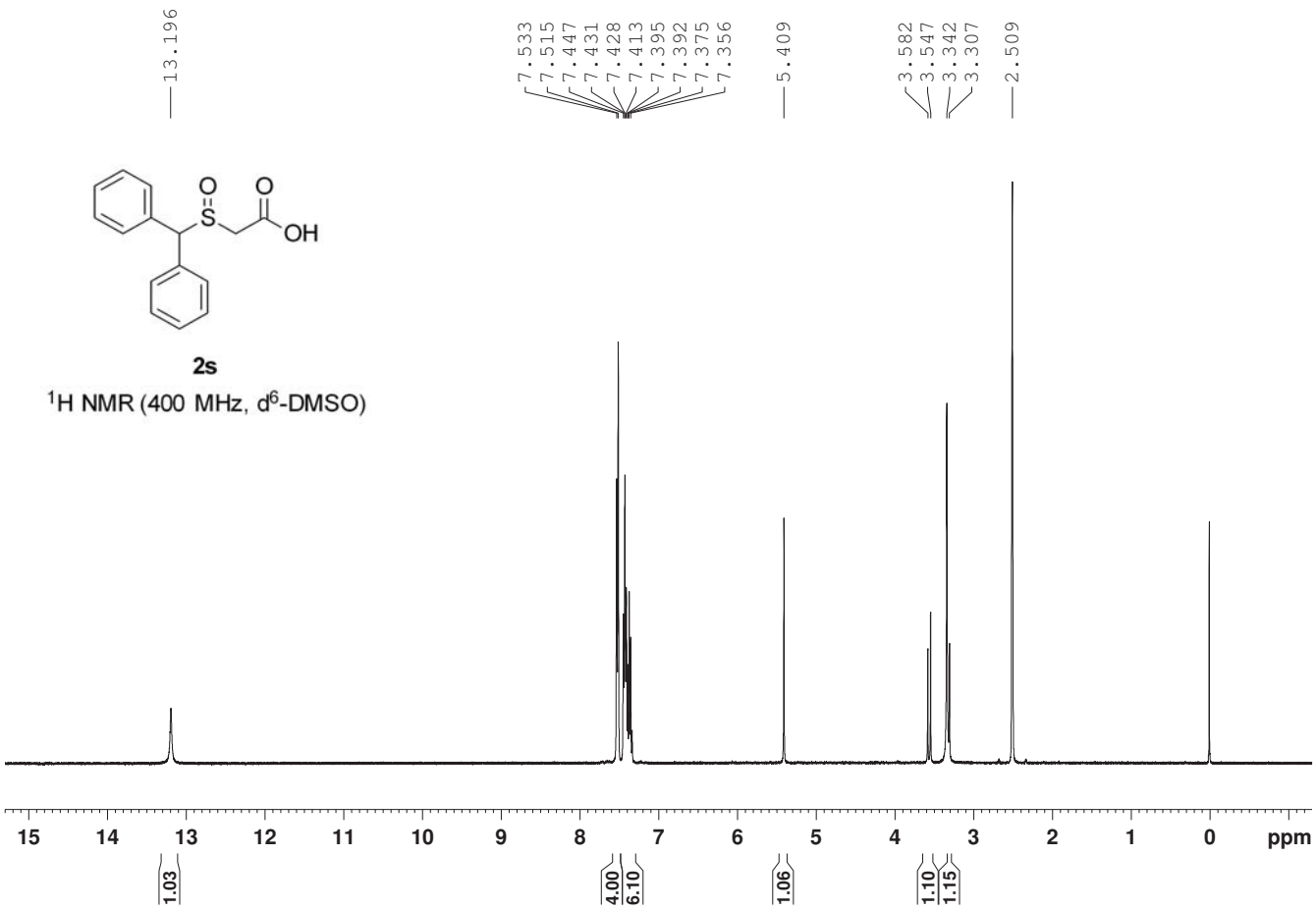
2r

^{1}H NMR (400 MHz, d^{6}-DMSO)



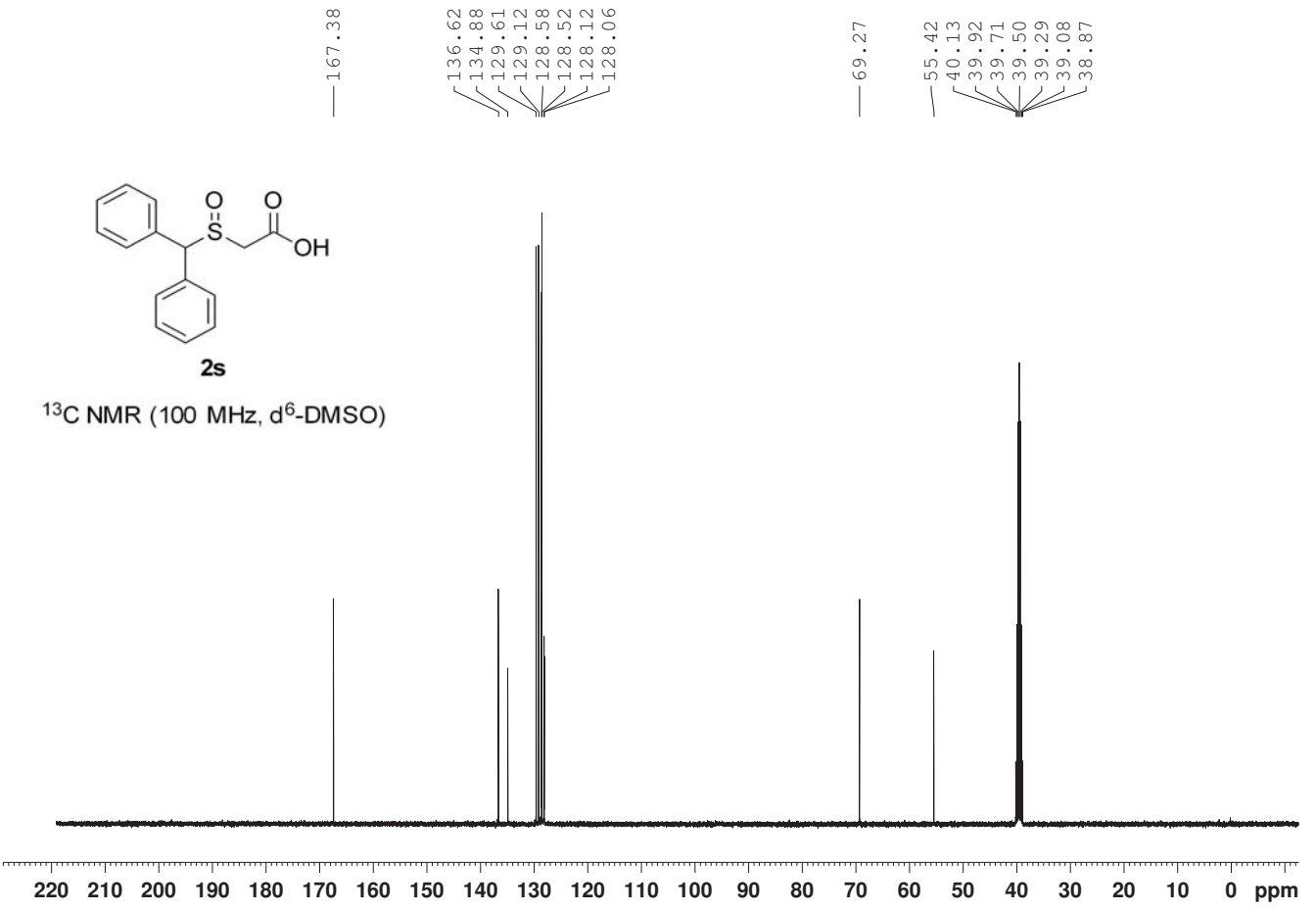
2r

^{13}C NMR (100 MHz, d^{6}-DMSO)



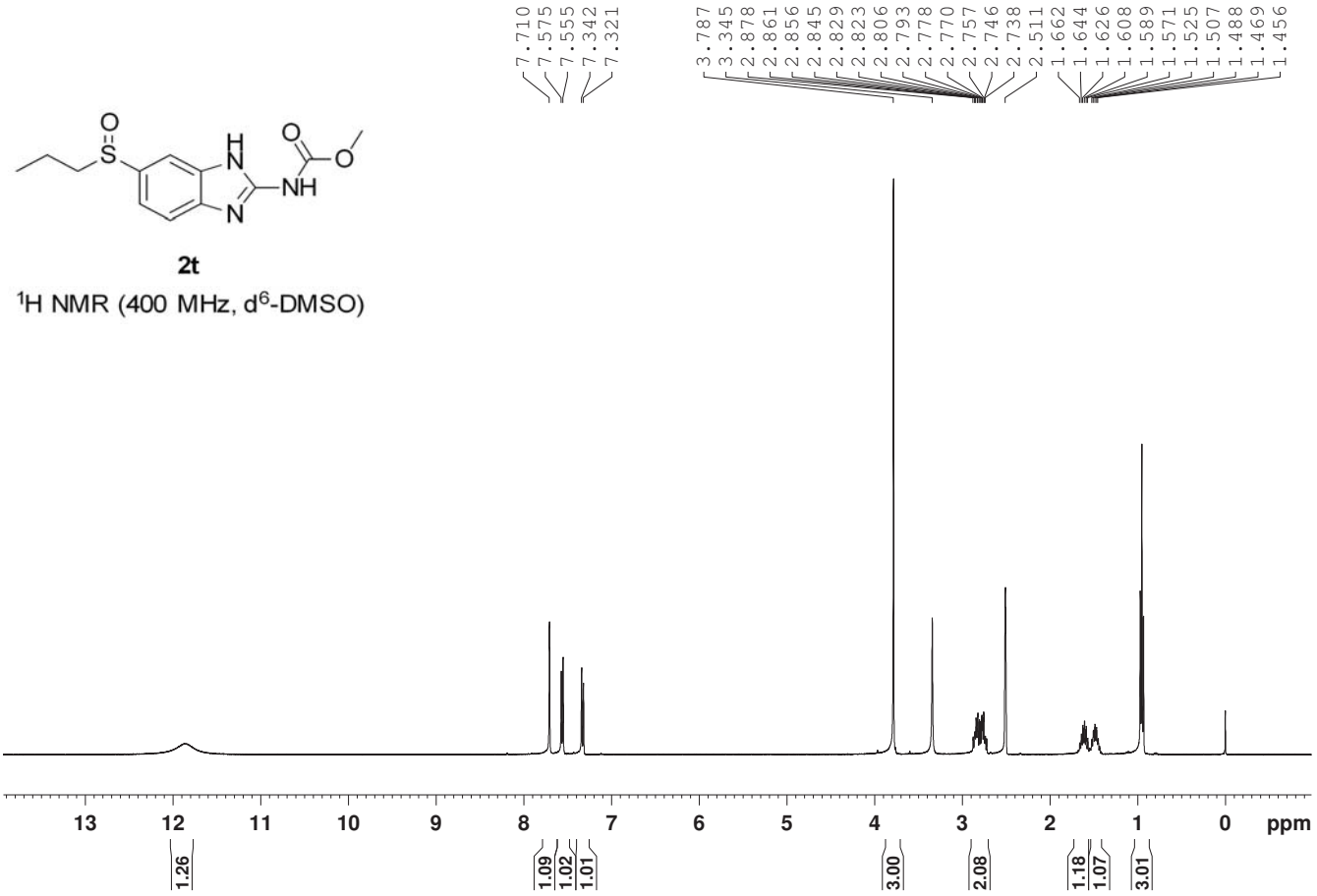
2s

^{1}H NMR (400 MHz, d^{6}-DMSO)



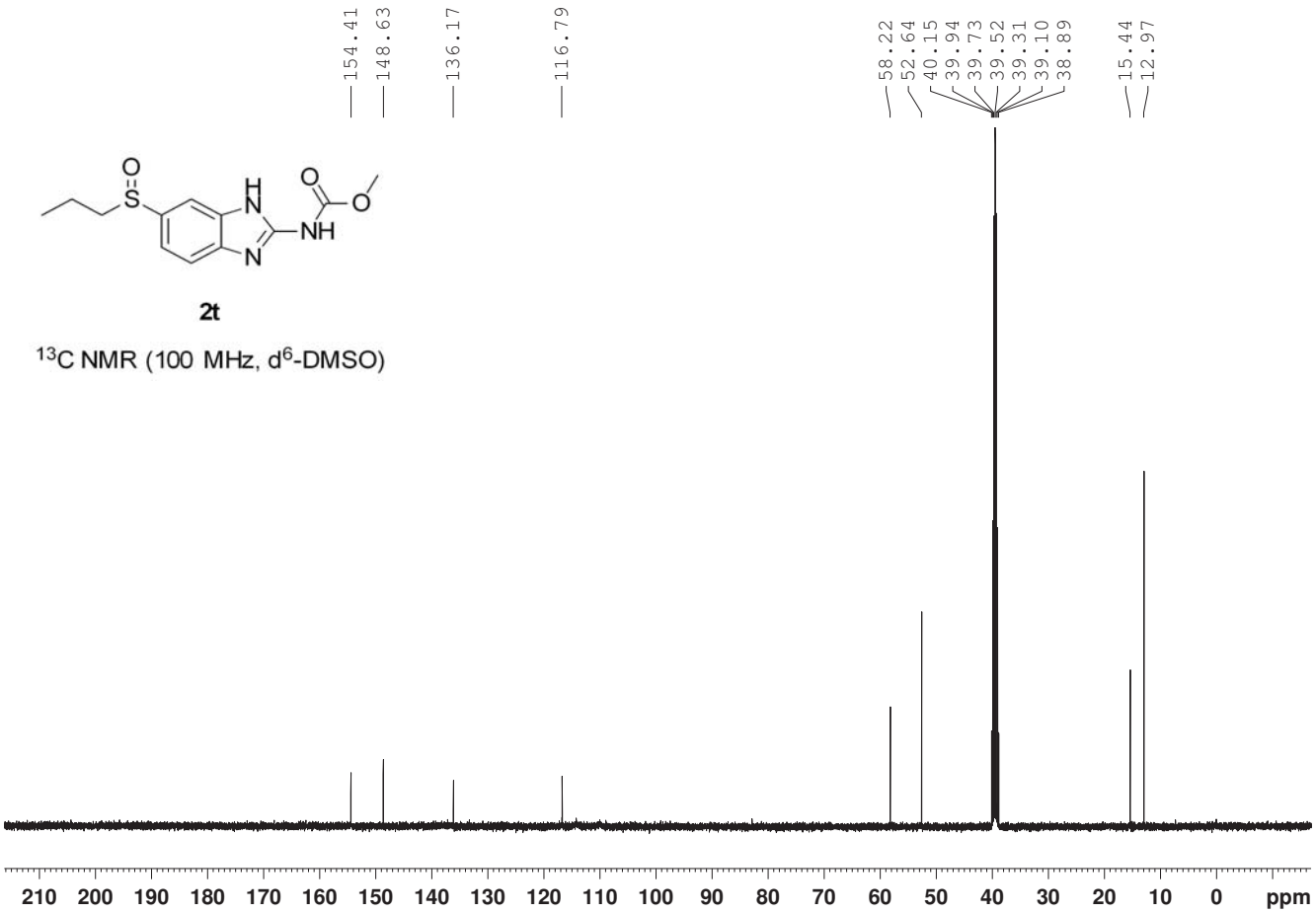
2s

^{13}C NMR (100 MHz, d^{6}-DMSO)



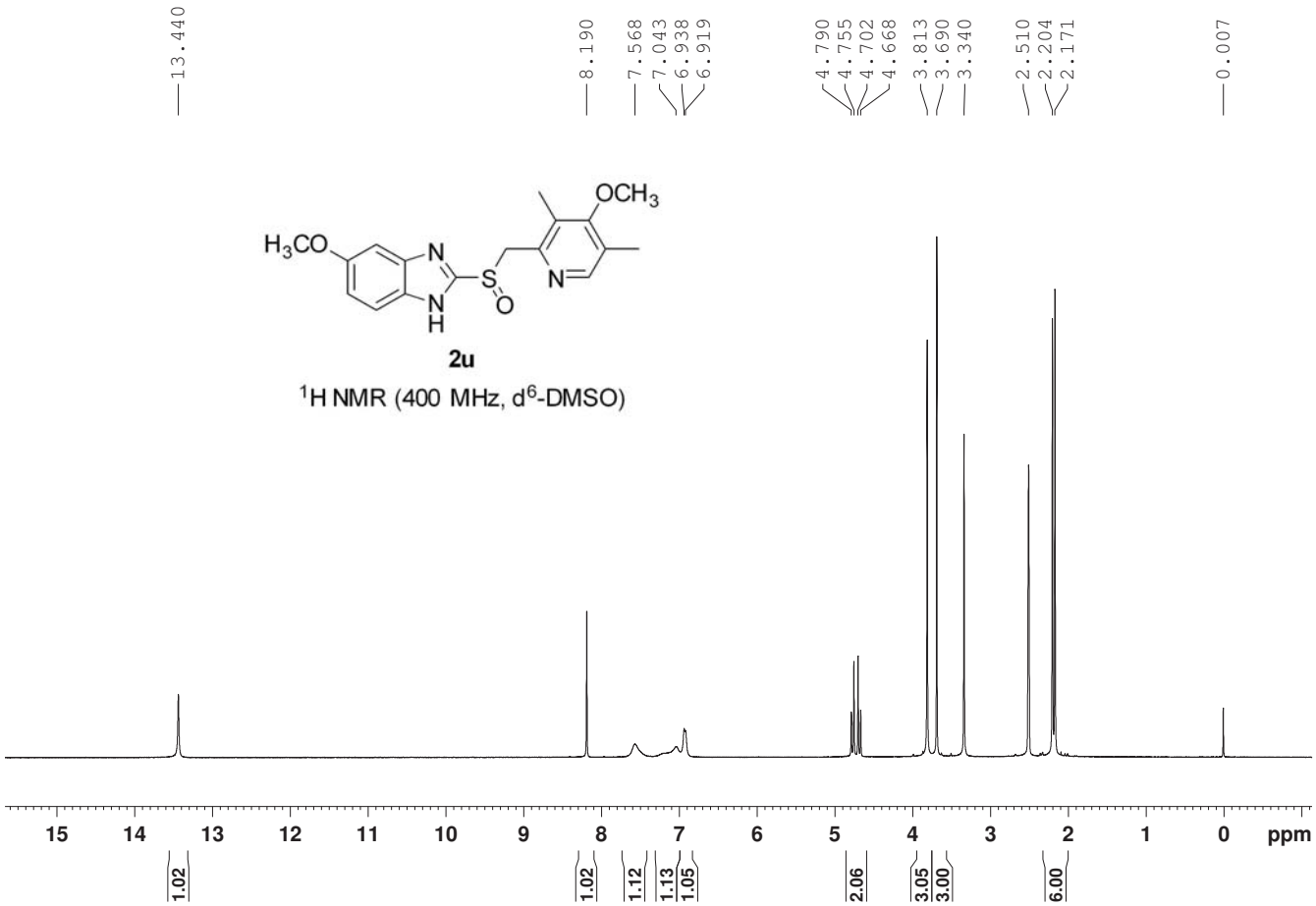
2t

^{1}H NMR (400 MHz, d^{6}-DMSO)



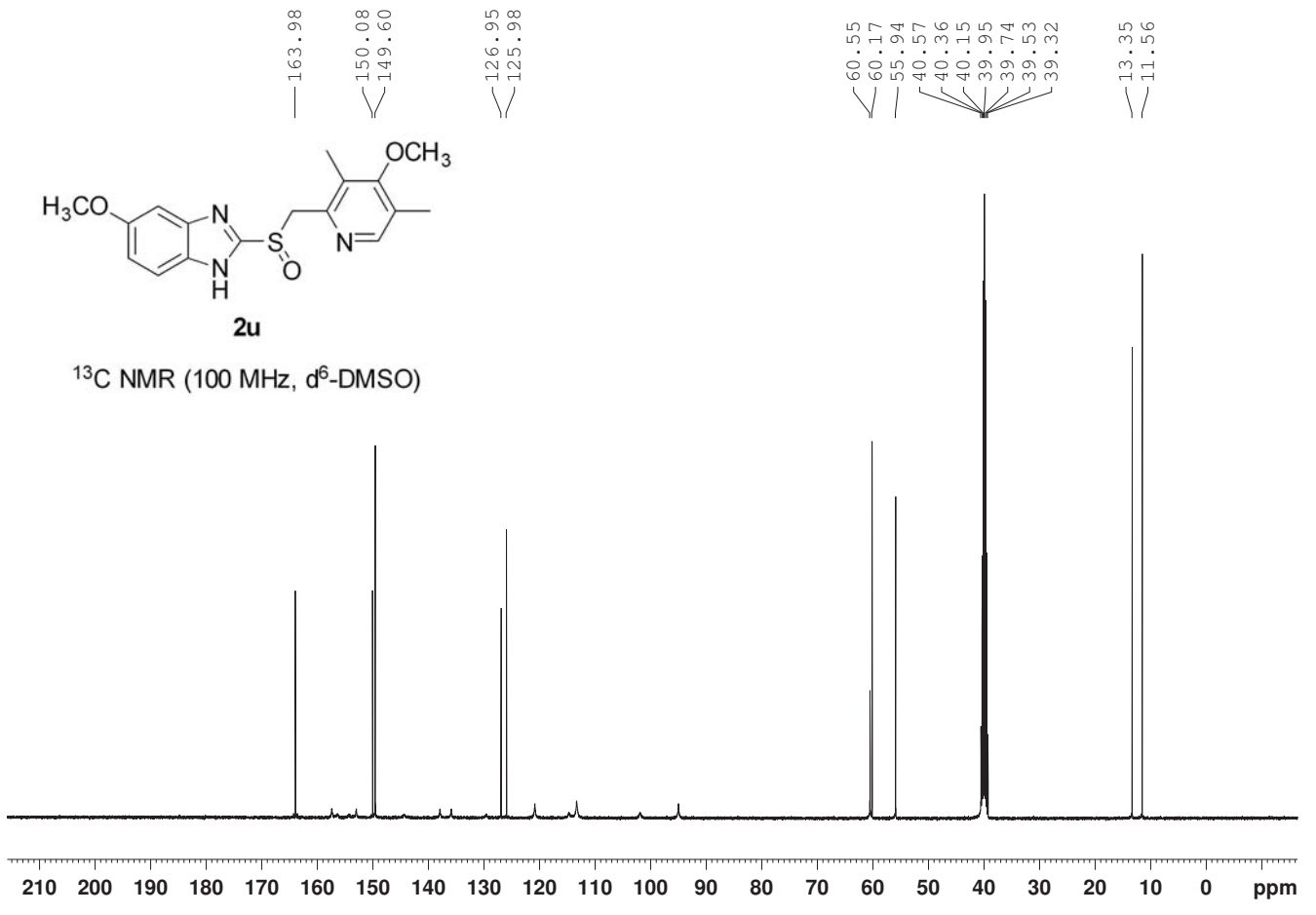
2t

^{13}C NMR (100 MHz, d^{6}-DMSO)



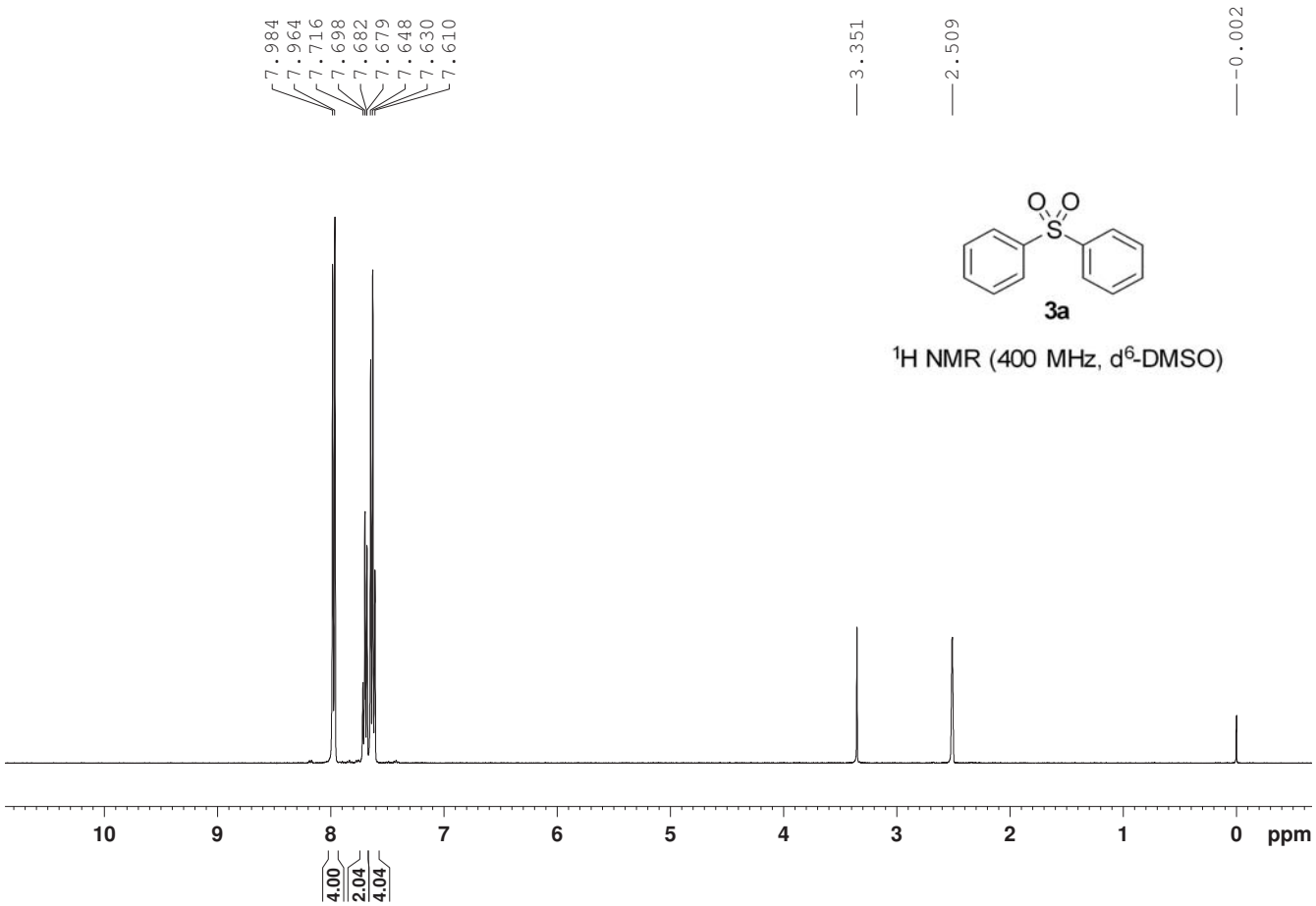
2u

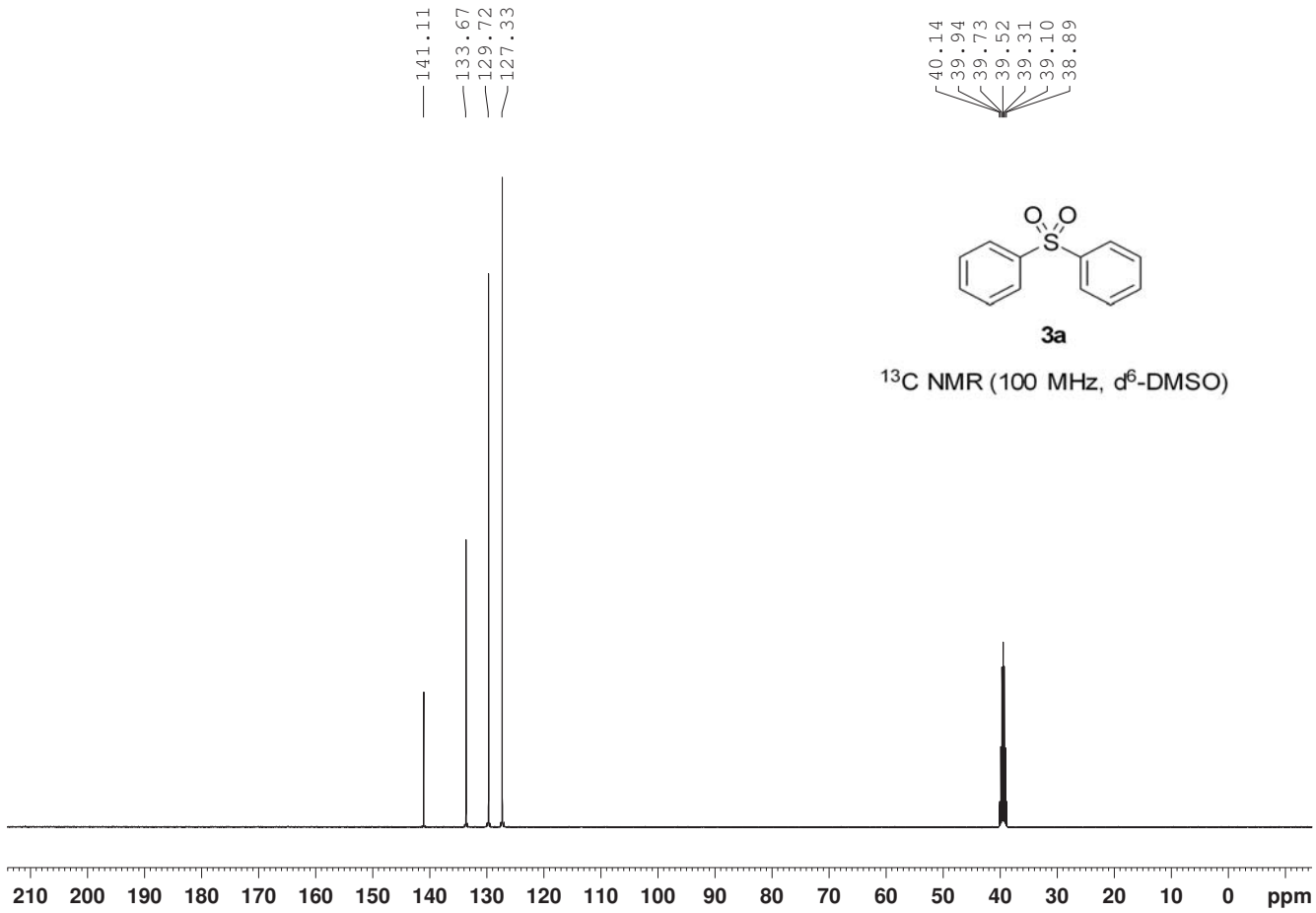
^{1}H NMR (400 MHz, d^{6}-DMSO)

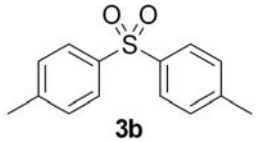


2u

^{13}C NMR (100 MHz, d^{6}-DMSO)

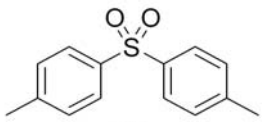

7.984
7.964
7.716
7.698
7.682
7.679
7.648
7.630
7.610
3.351
2.509
0.002
3a
1H NMR (400 MHz, d6-DMSO)
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
2.04
4.04


141.11
133.67
129.72
127.33
40.14
39.94
39.73
39.52
39.31
39.10
38.89
3a
13C NMR (100 MHz, d6-DMSO)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



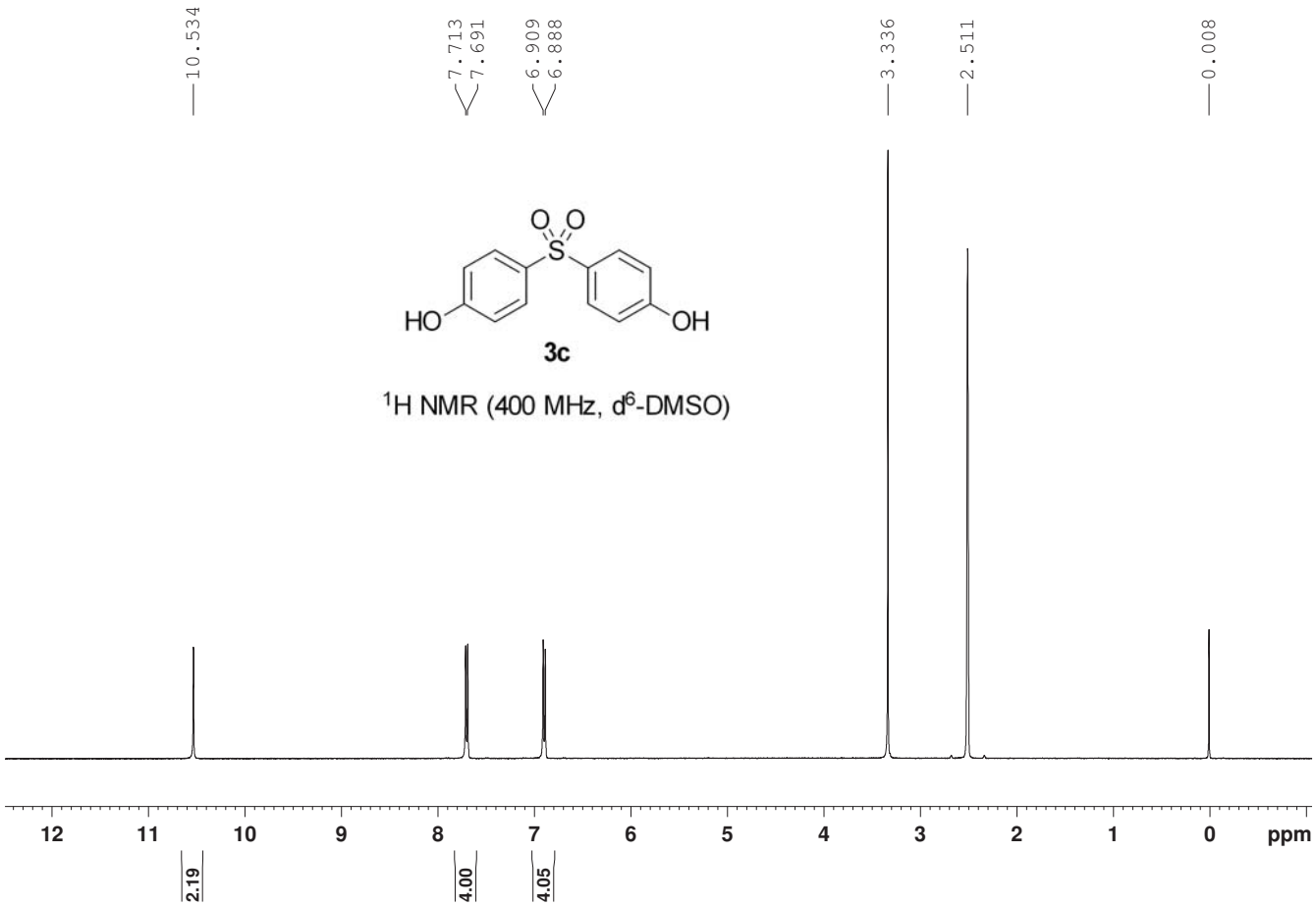
3b

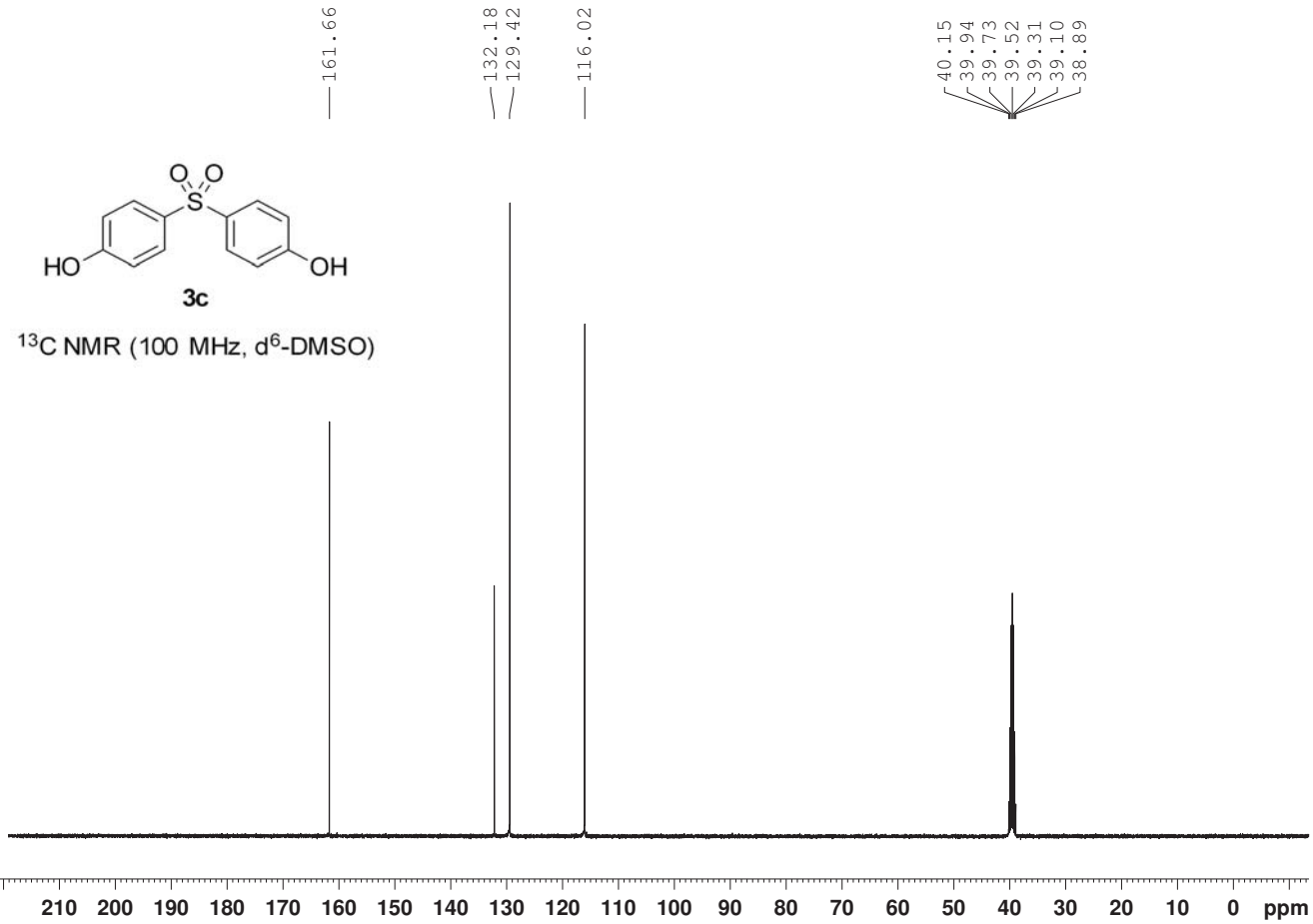
^{1}H NMR (400 MHz, d^{6}-DMSO)

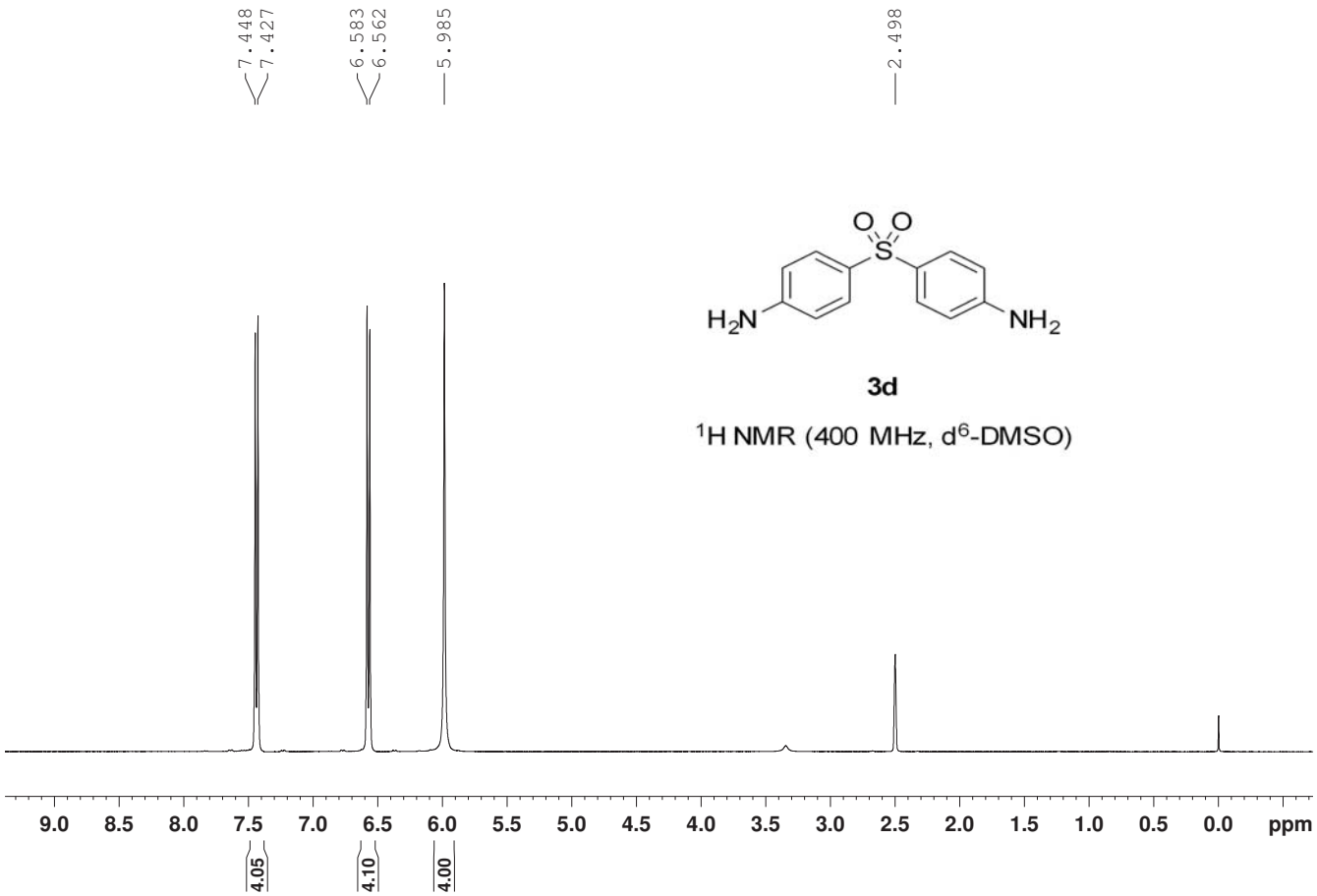


3b

^{13}C NMR (100 MHz, d^{6}-DMSO)

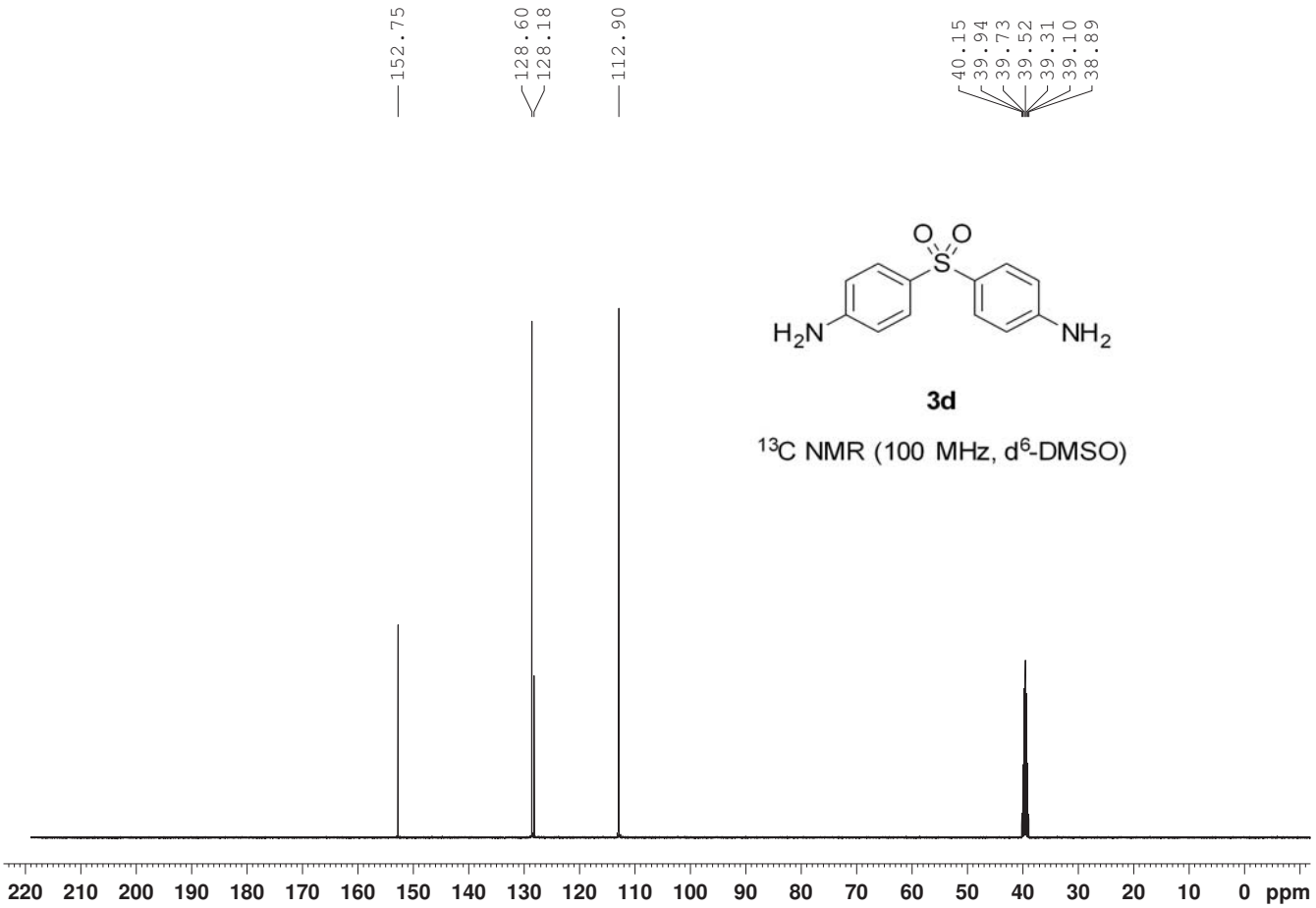

10.534
7.713
7.691
6.909
6.888
3.336
2.511
0.008
HO
OH
3c
1H NMR (400 MHz, d6-DMSO)
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.19
4.00
4.05


161.66
132.18
129.42
116.02
40.15
39.94
39.73
39.52
39.31
39.10
38.89
HO
OH
3c
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



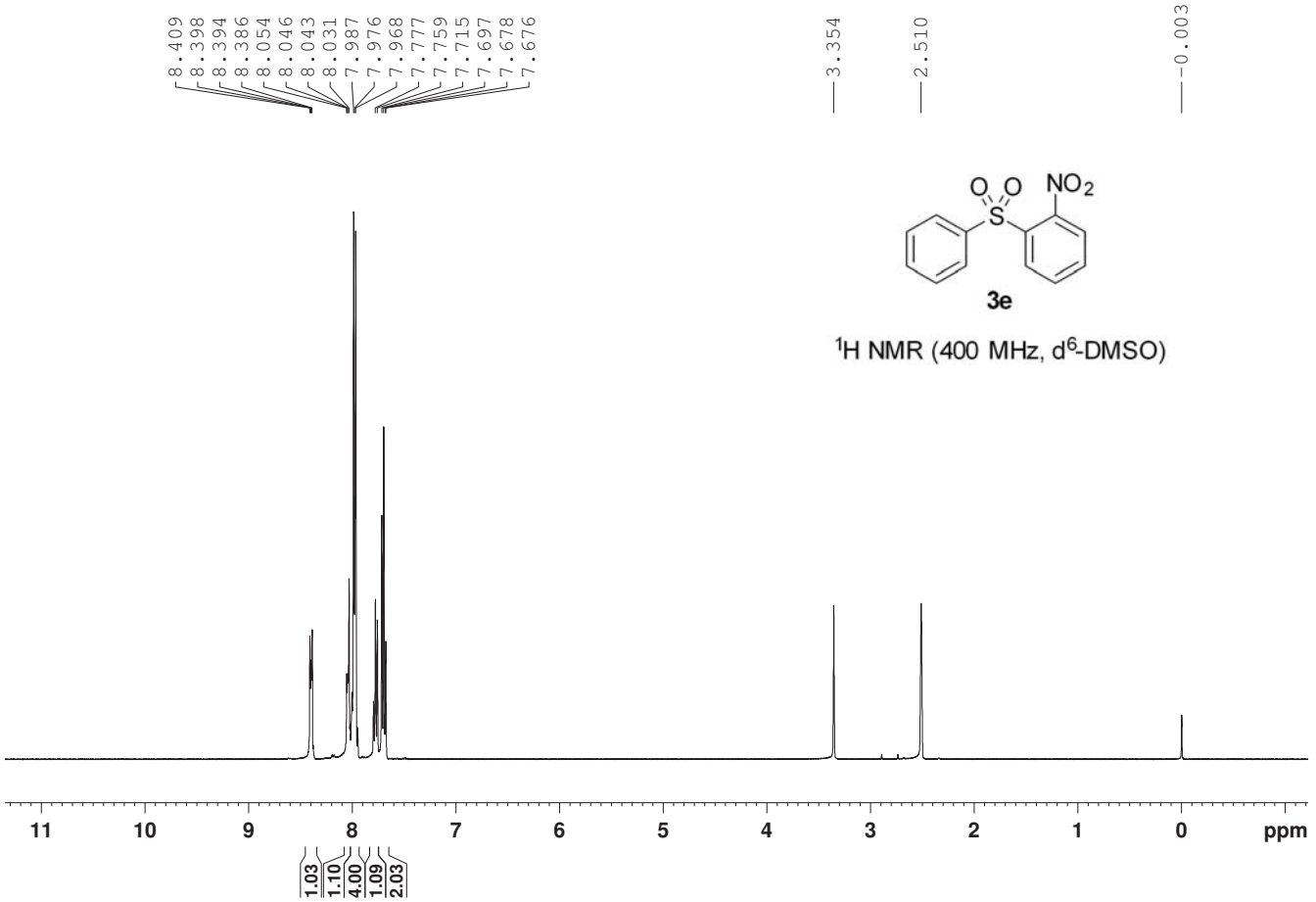
3d

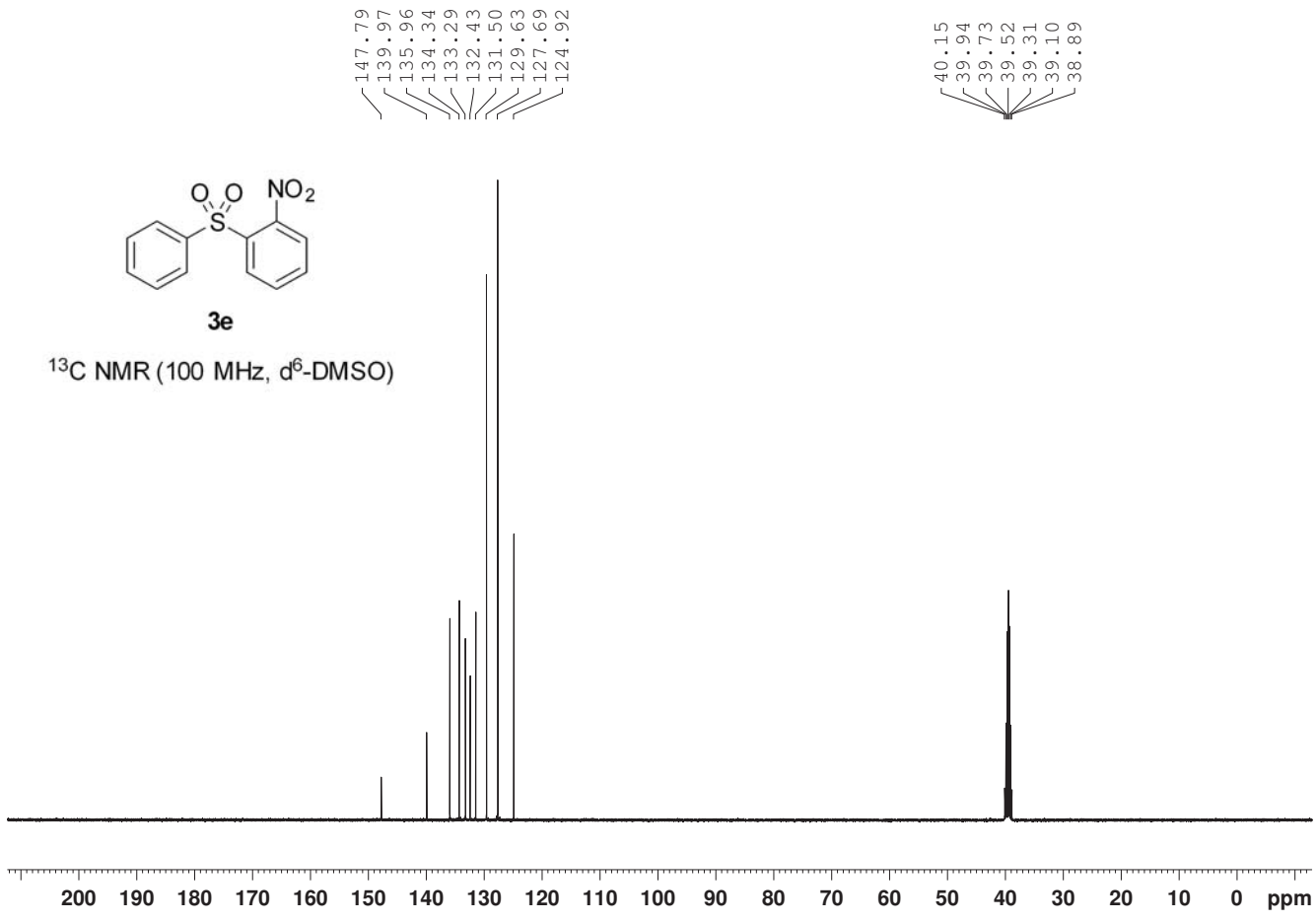
^{1}H NMR (400 MHz, d^{6}-DMSO)

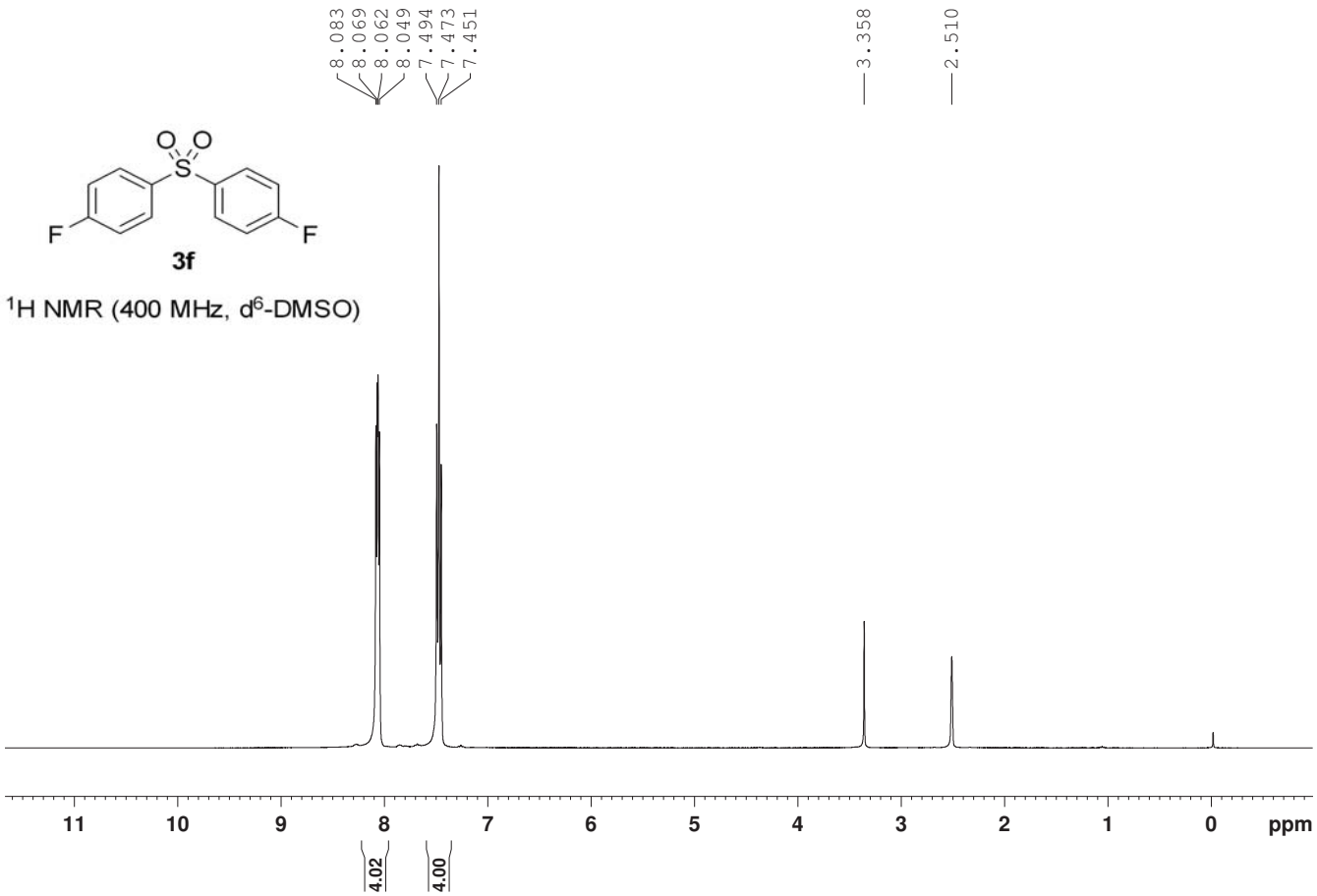


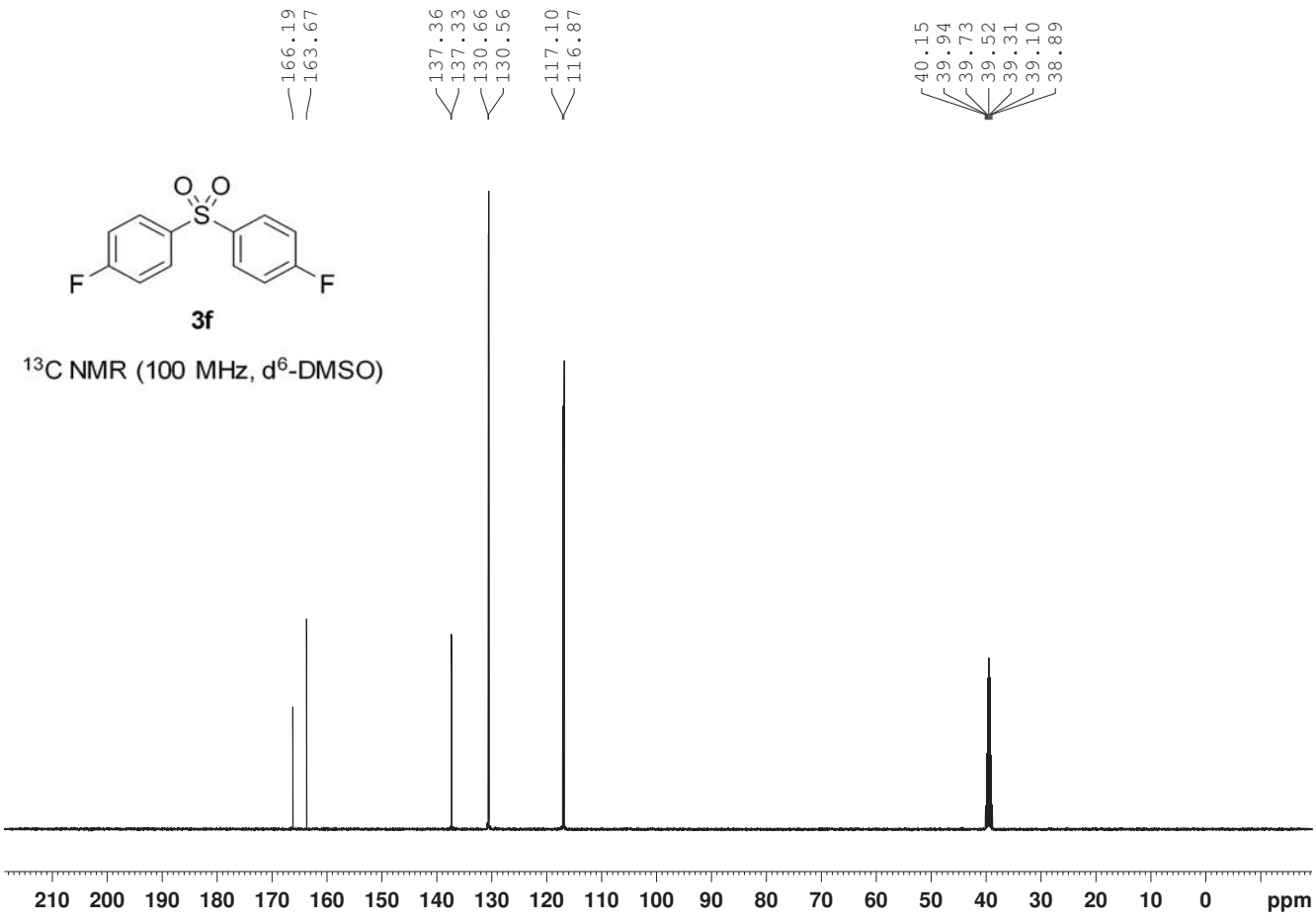
3d

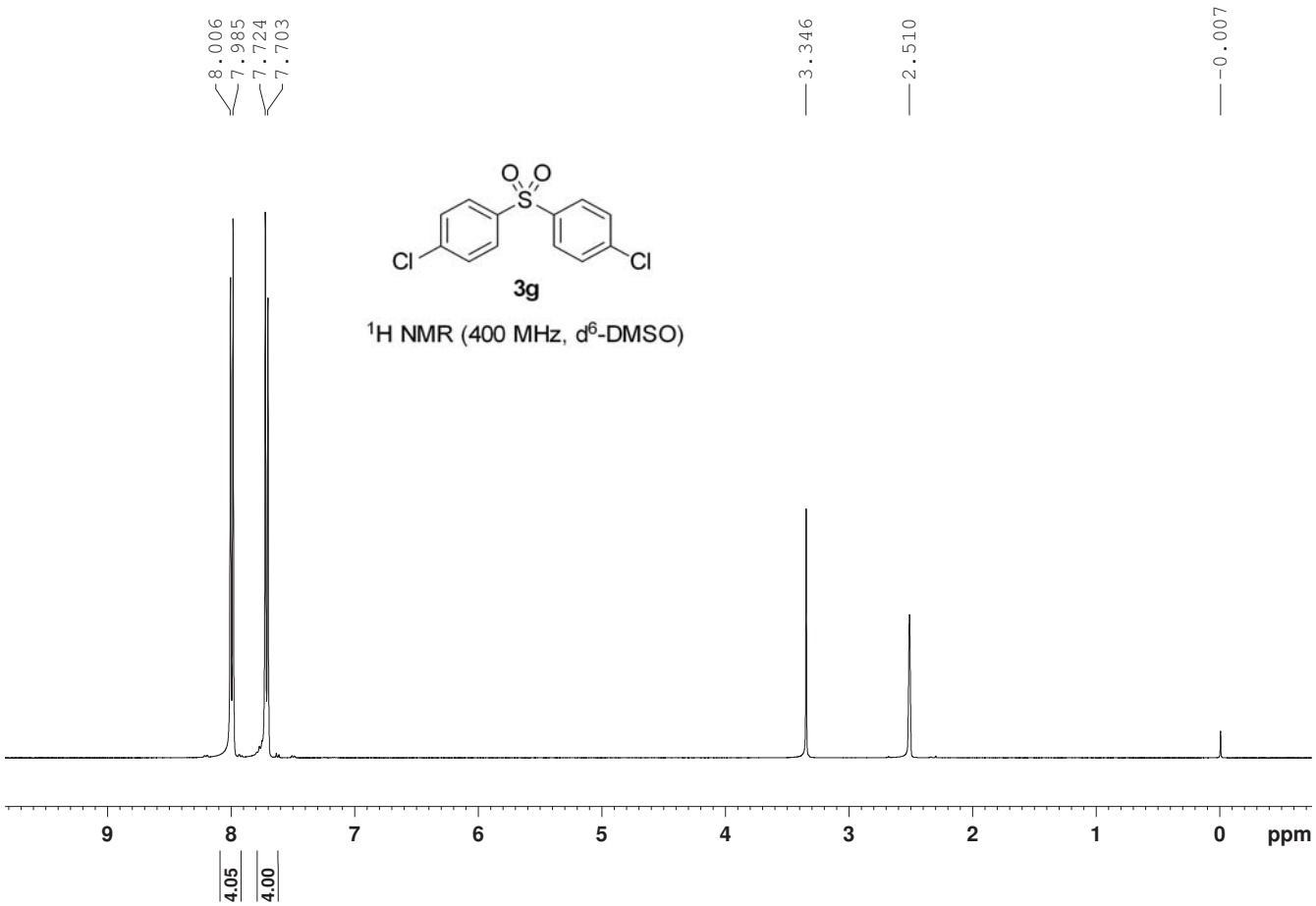
^{13}C NMR (100 MHz, d^{6}-DMSO)

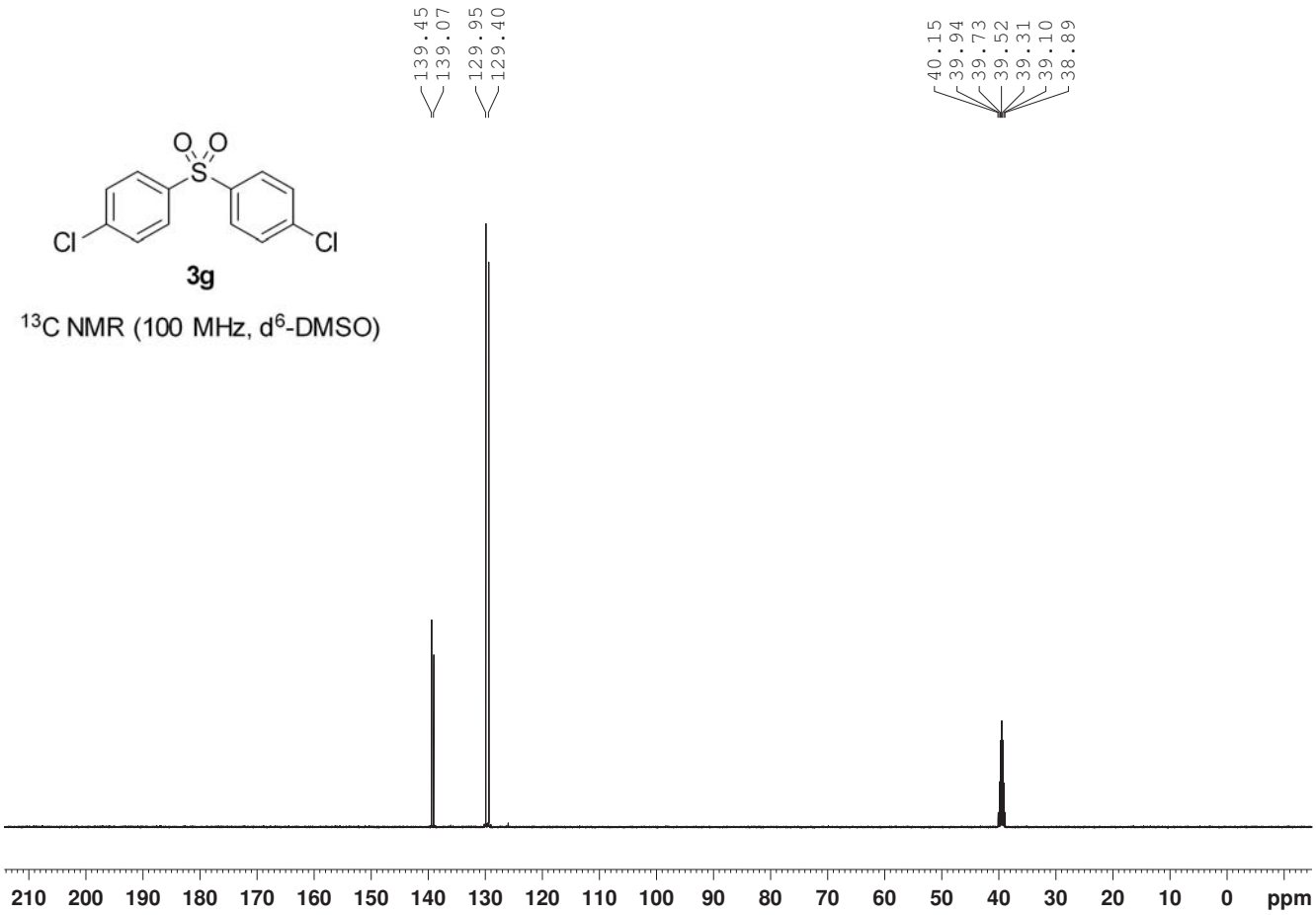

8.409
8.398
8.394
8.386
8.054
8.046
8.043
8.031
7.987
7.976
7.968
7.777
7.759
7.715
7.697
7.678
7.676
3.354
2.510
0.003
O
O
S
NO2
3e
1H NMR (400 MHz, d6-DMSO)
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.10
4.00
1.09
2.03

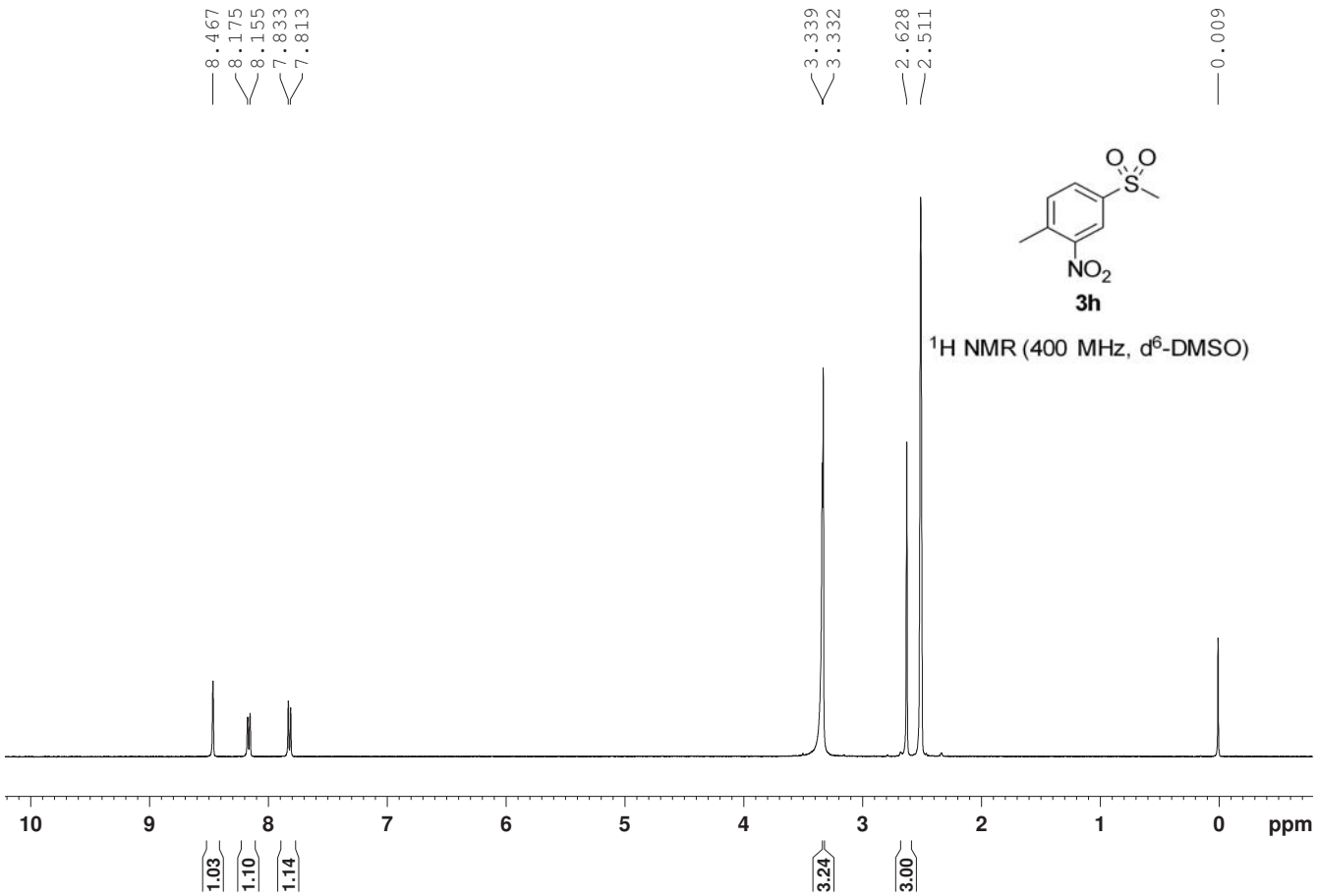

147.79
139.97
135.96
134.34
133.29
132.43
131.50
129.63
127.69
124.92
40.15
39.94
39.73
39.52
39.31
39.10
38.89
O
O
S
NO2
3e
13C NMR (100 MHz, d6-DMSO)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

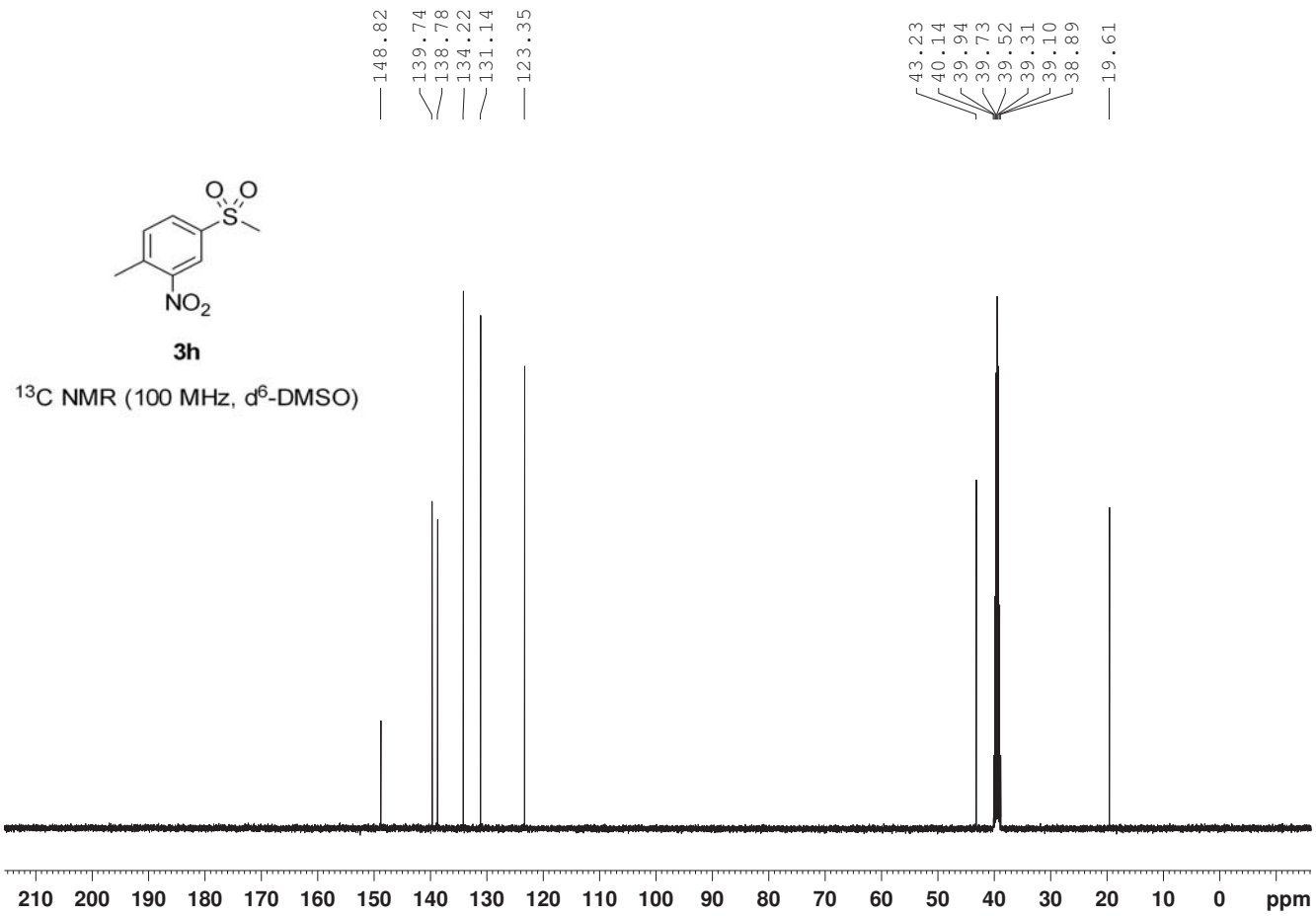

8.083
8.069
8.062
8.049
7.494
7.473
7.451
3.358
2.510
3f
1H NMR (400 MHz, d6-DMSO)
11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.02
4.00

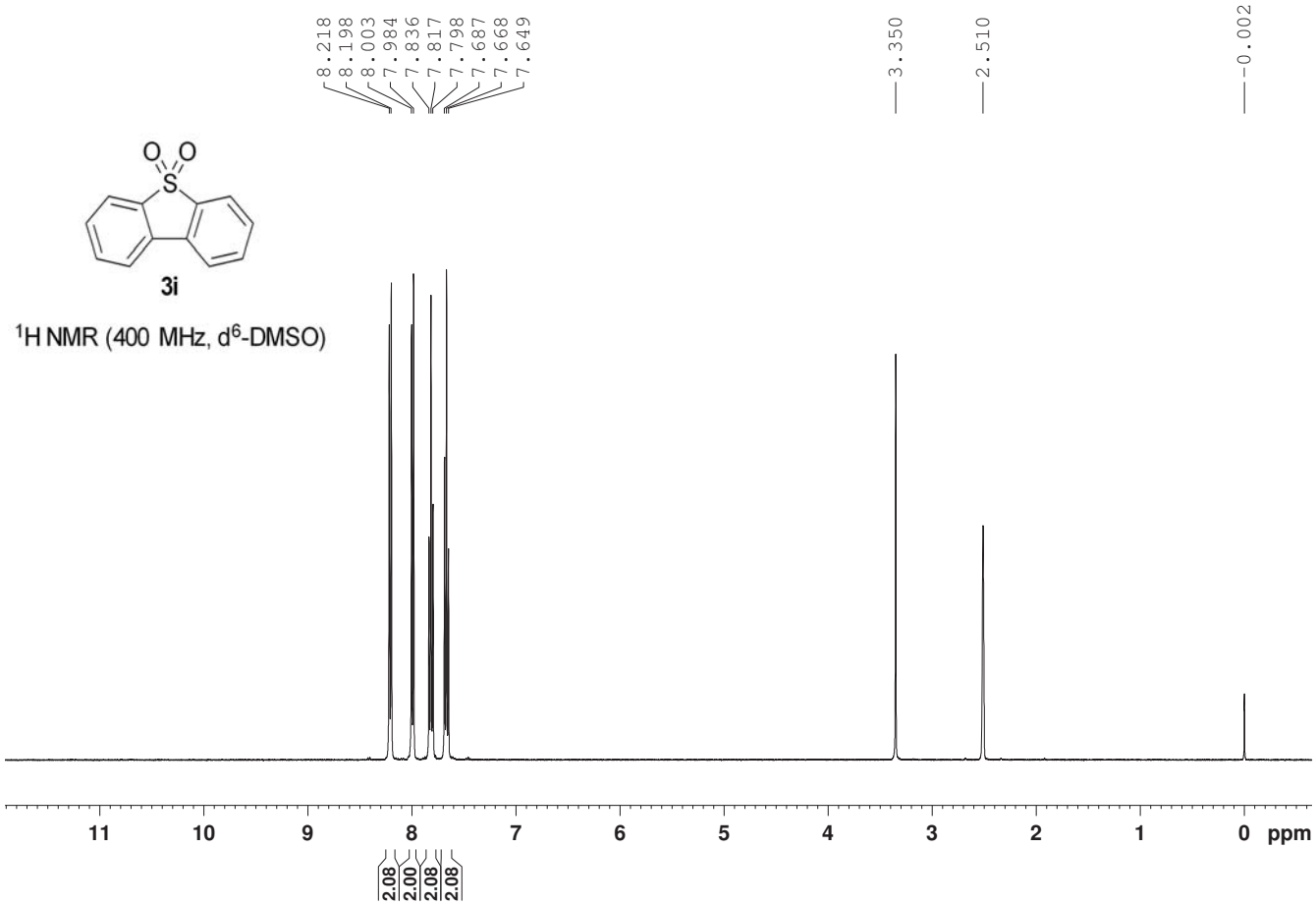

166.19
163.67
137.36
137.33
130.66
130.56
117.10
116.87
40.15
39.94
39.73
39.52
39.31
39.10
38.89
3f
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

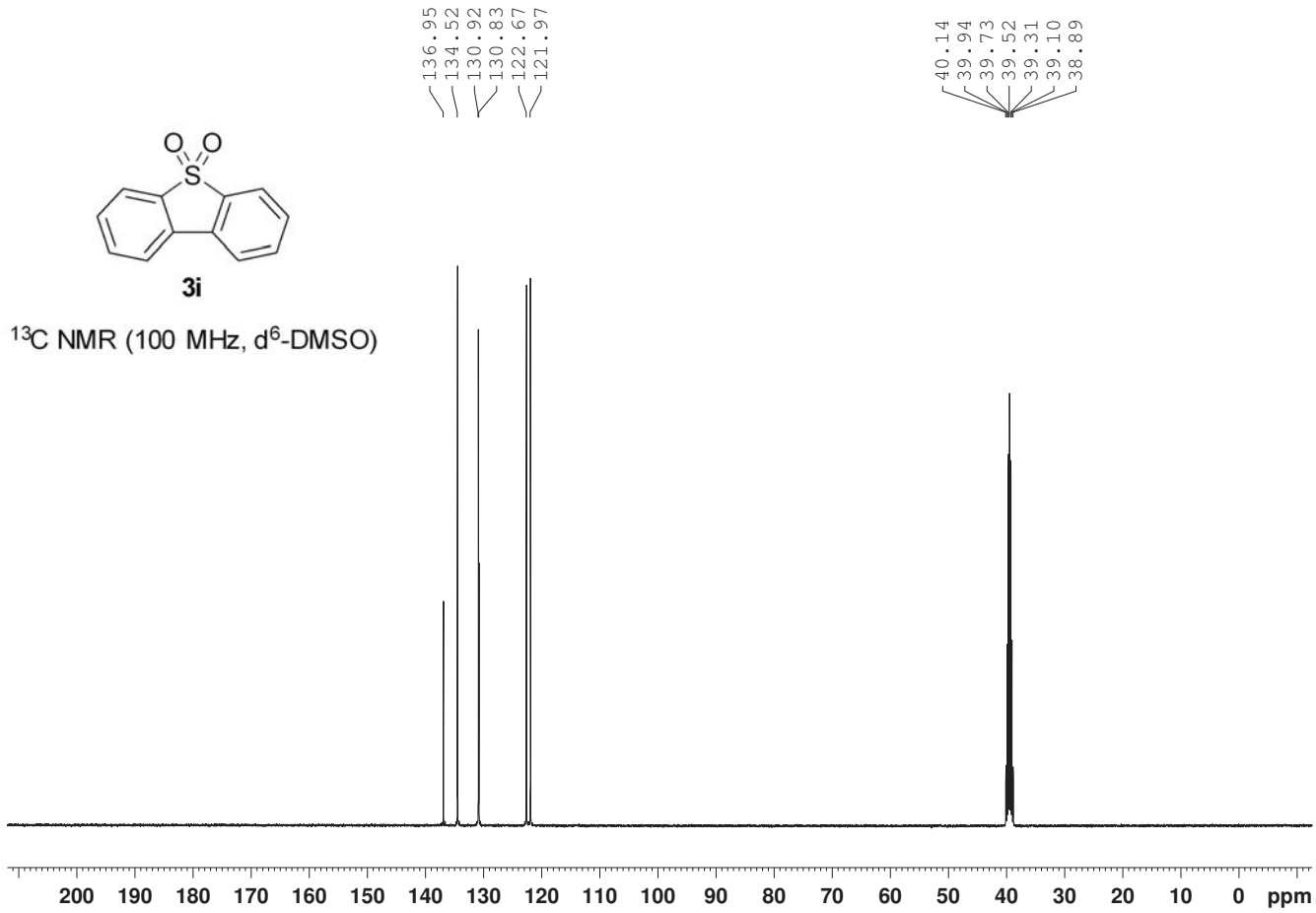

8.006
7.985
7.724
7.703
3.346
2.510
0.007
Cl
Cl
3g
1H NMR (400 MHz, d6-DMSO)
9
8
7
6
5
4
3
2
1
0
ppm
4.05
4.00

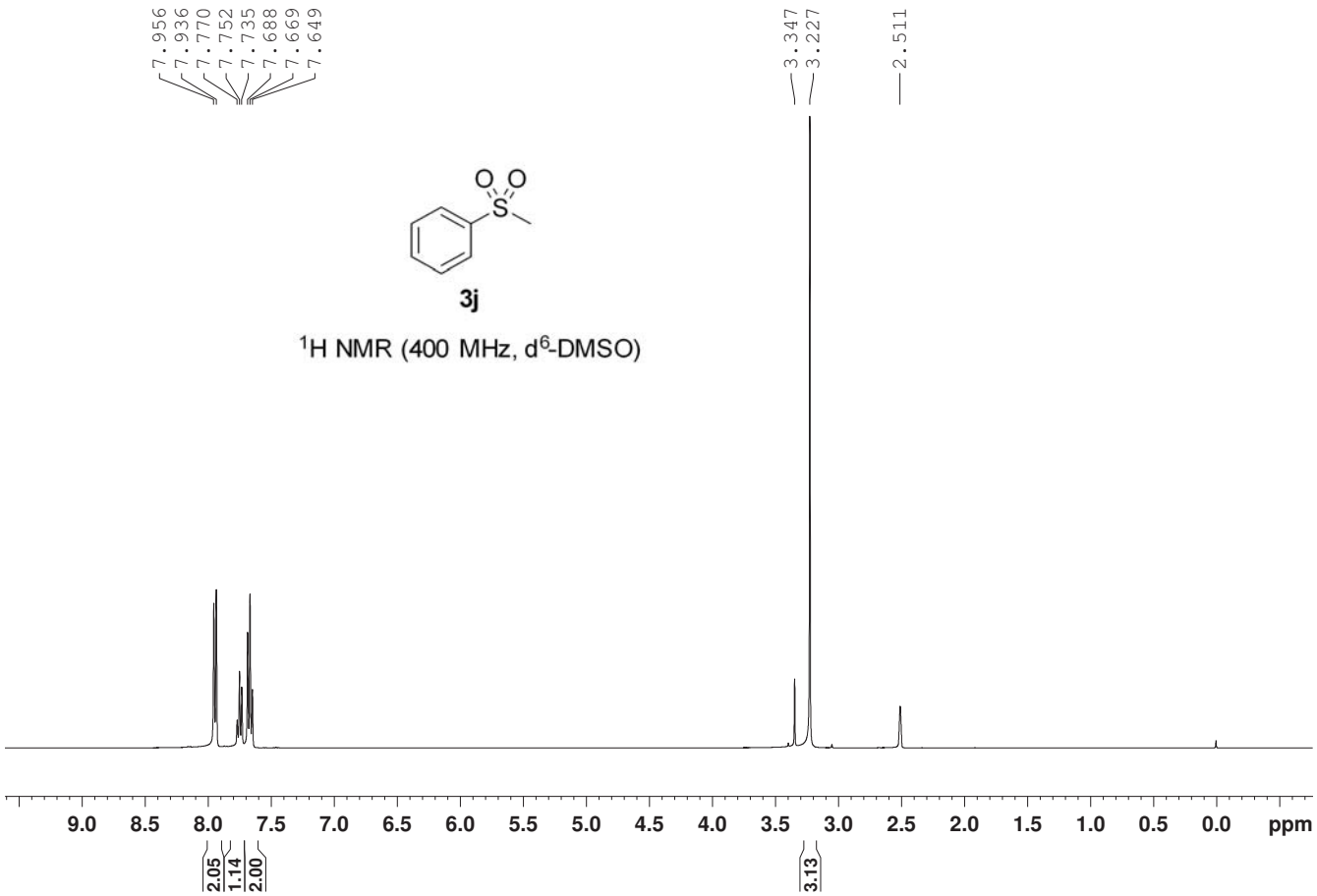

139.45
139.07
129.95
129.40
40.15
39.94
39.73
39.52
39.31
39.10
38.89
Cl
Cl
3g
13C NMR (100 MHz, d6-DMSO)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.467
8.175
8.155
7.833
7.813
3.339
3.332
2.628
2.511
0.009
O O
S
NO2
3h
1H NMR (400 MHz, d6-DMSO)
10 9 8 7 6 5 4 3 2 1 0 ppm
1.03
1.10
1.14
3.24
3.00


148.82
139.74
138.78
134.22
131.14
123.35
43.23
40.14
39.94
39.73
39.52
39.31
39.10
38.89
19.61
O O
S
NO2
3h
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

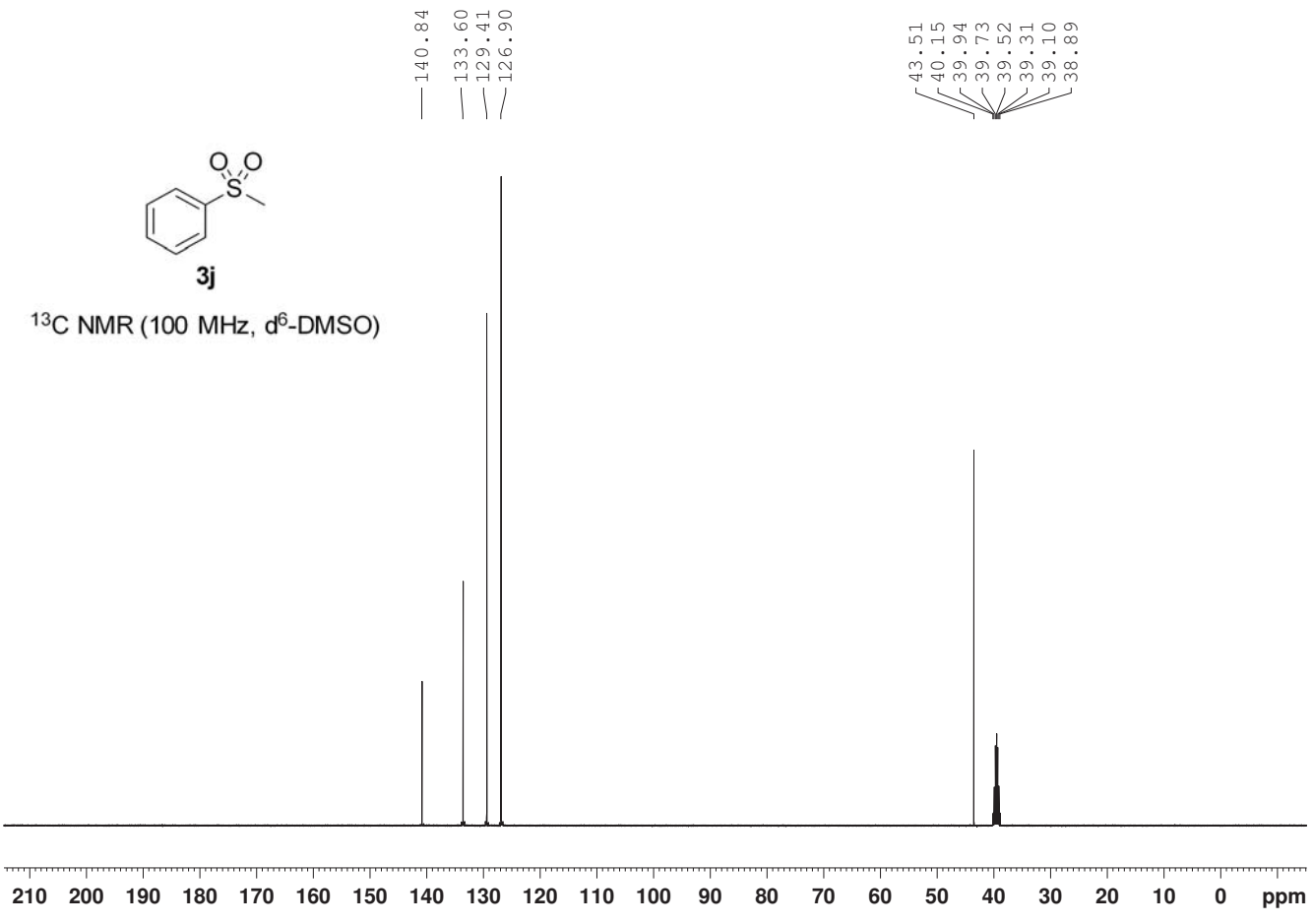

8.218
8.198
8.003
7.984
7.836
7.817
7.798
7.687
7.668
7.649
3.350
2.510
0.002
3i
1H NMR (400 MHz, d6-DMSO)
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.08
2.00
2.08
2.08


136.95
134.52
130.92
130.83
122.67
121.97
40.14
39.94
39.73
39.52
39.31
39.10
38.89
3i
13C NMR (100 MHz, d6-DMSO)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



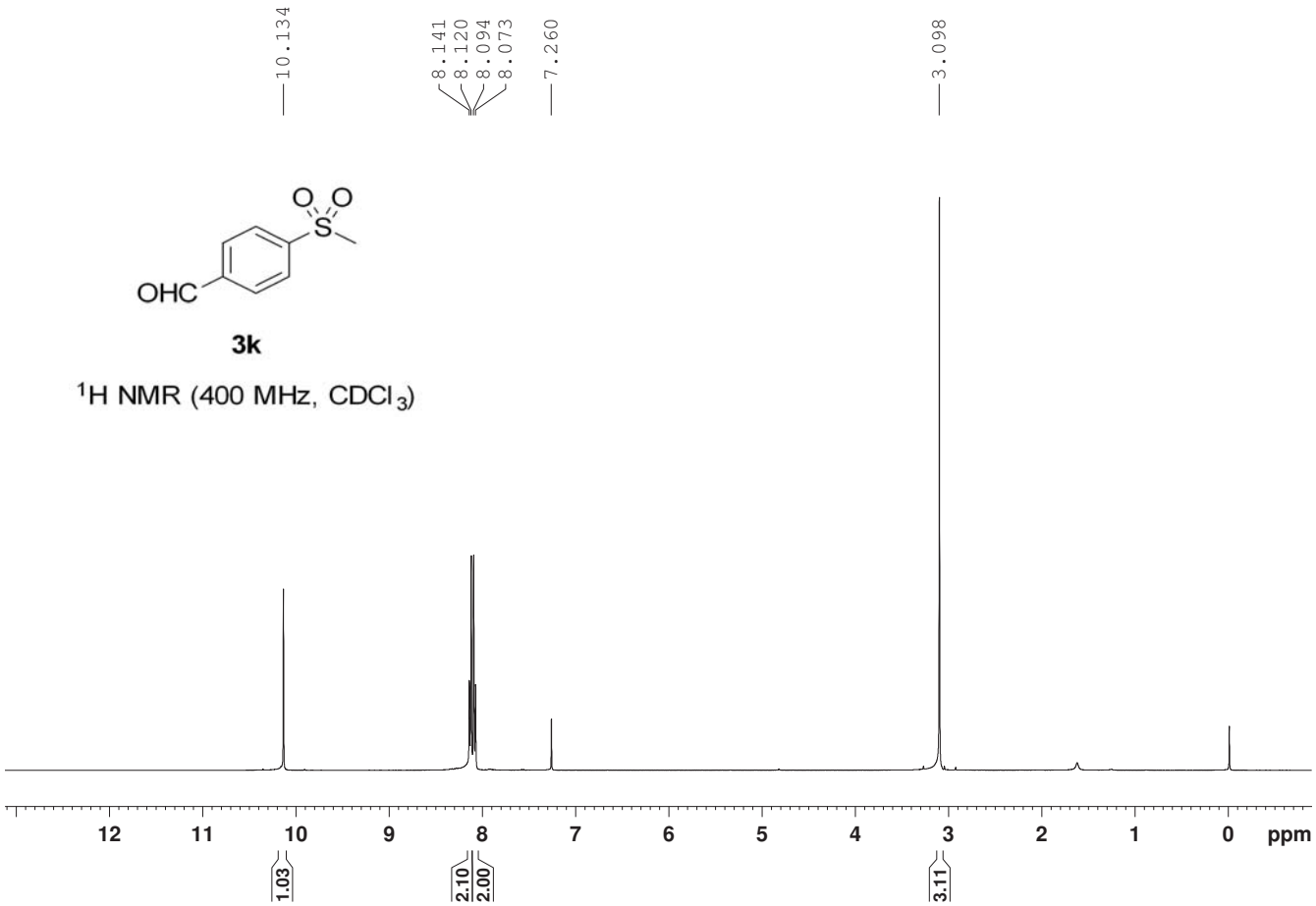
3j

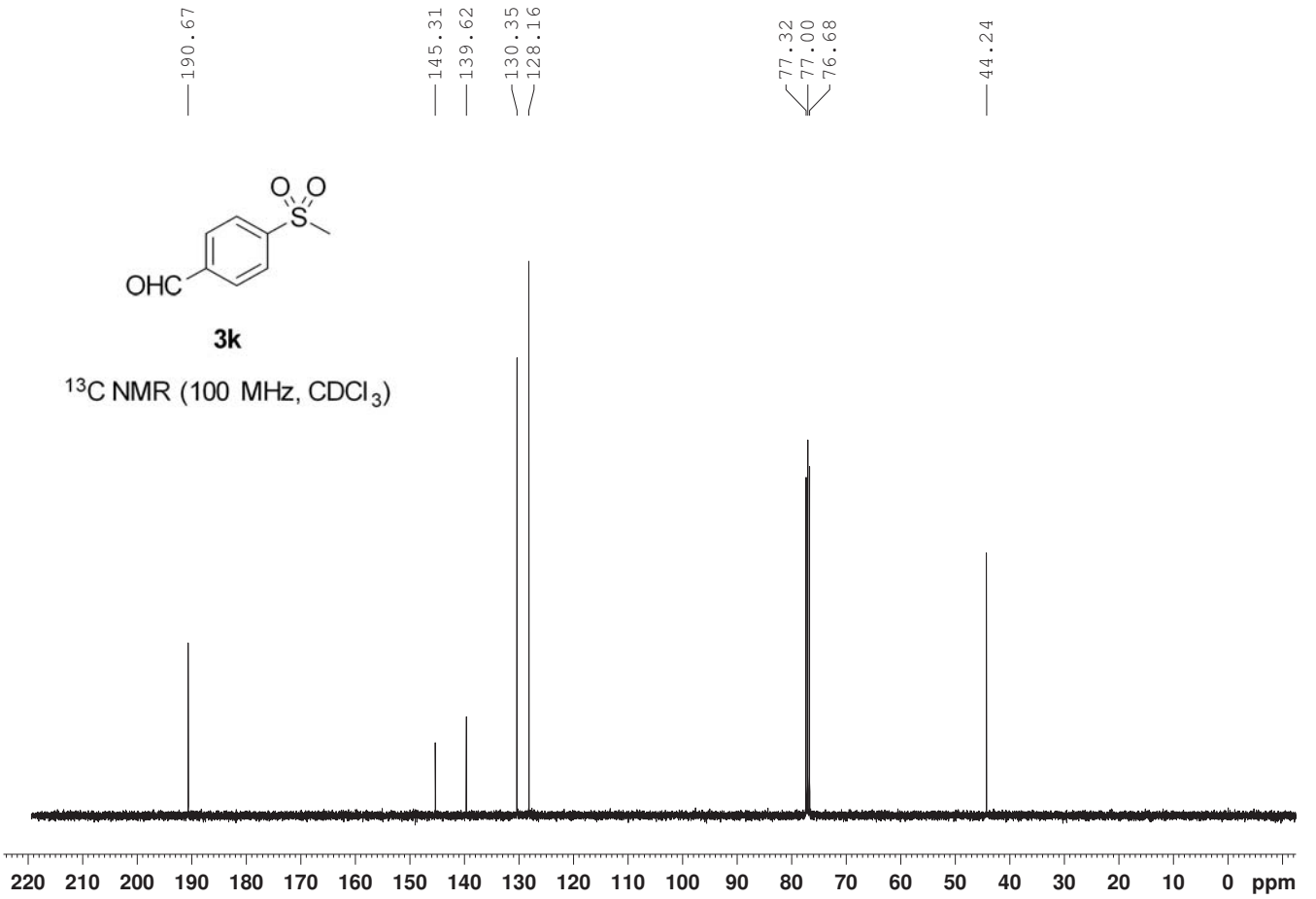
^{1}H NMR (400 MHz, d^{6}-DMSO)

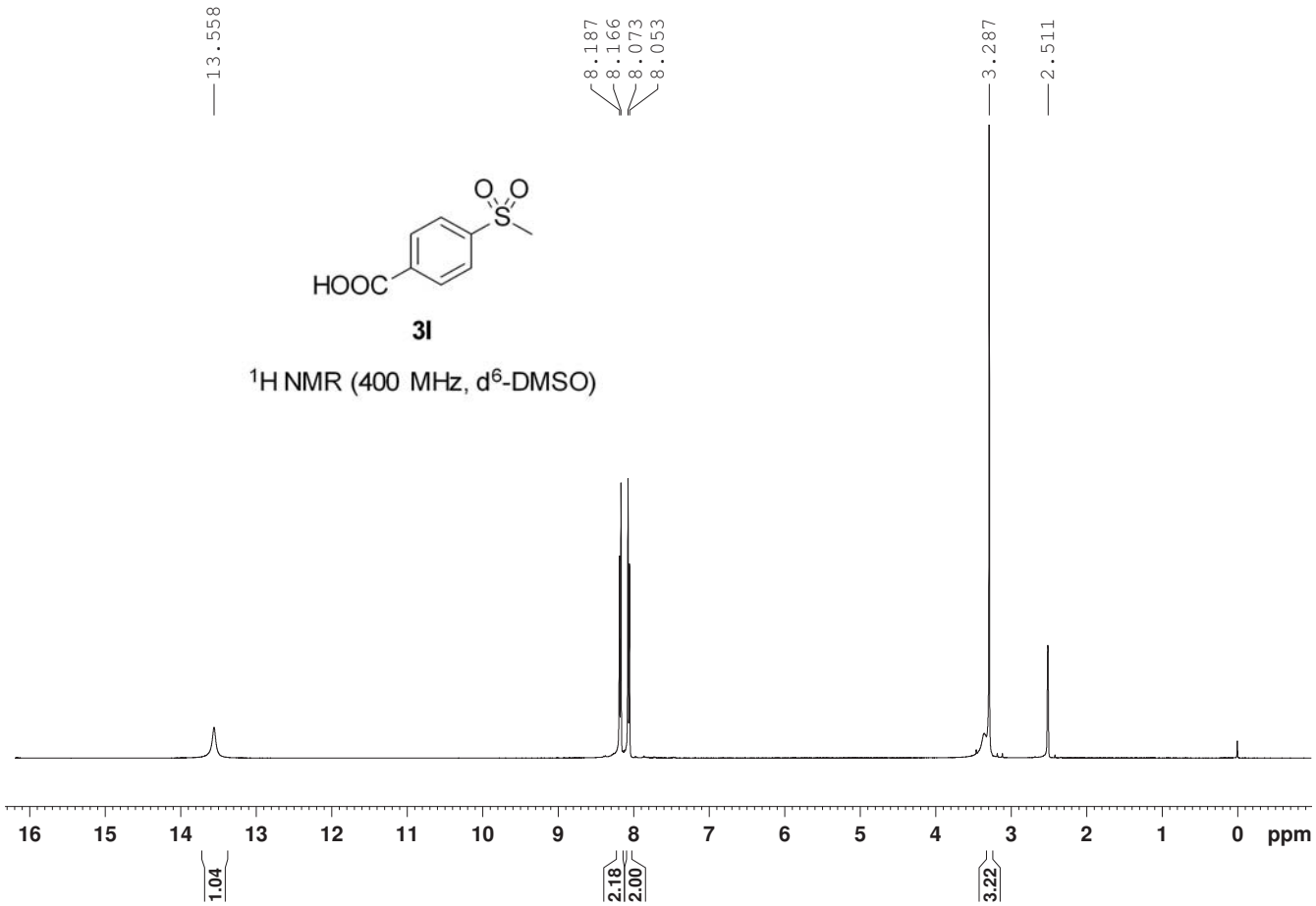


3j

^{13}C NMR (100 MHz, d^{6}-DMSO)

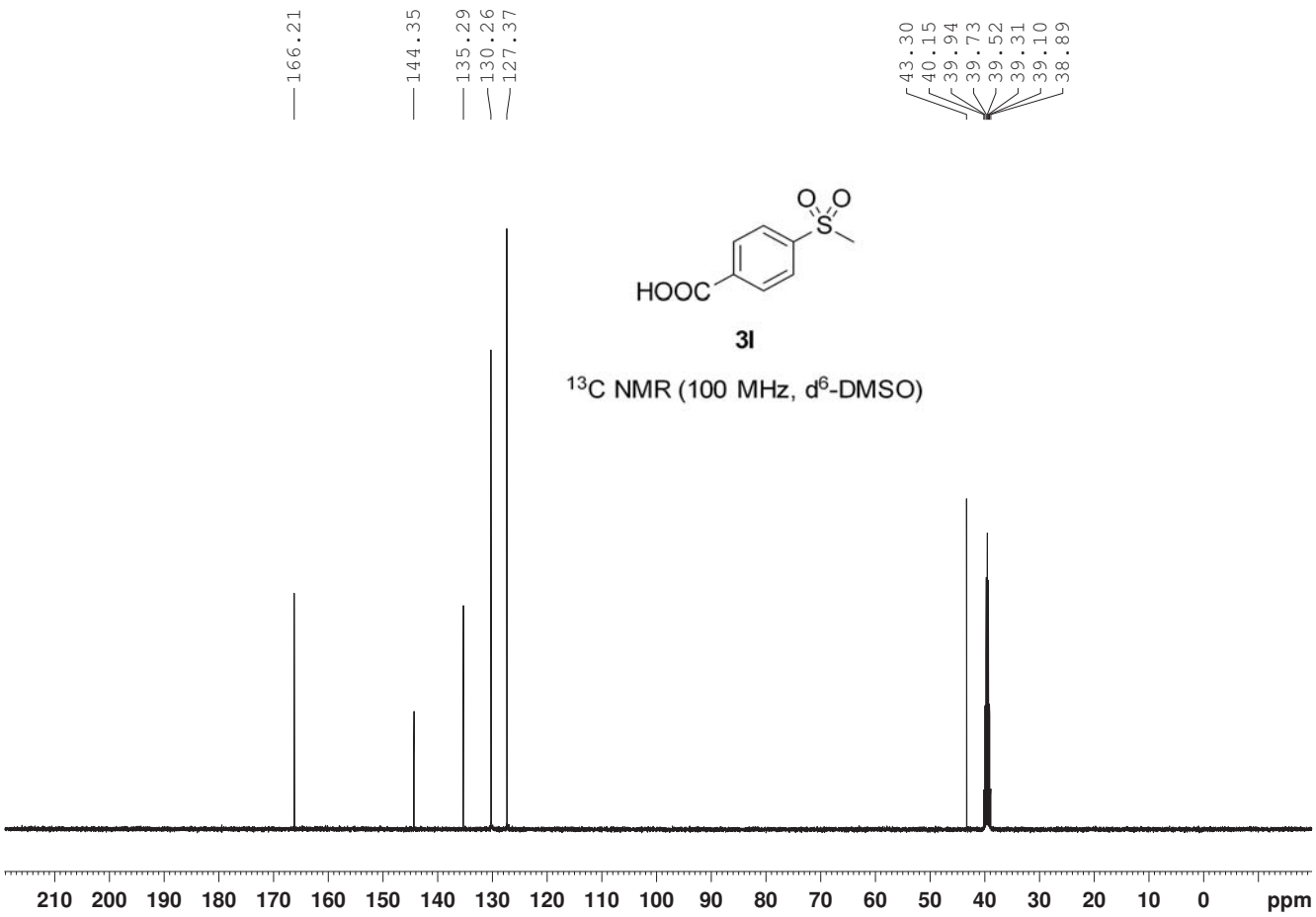

10.134
8.141
8.120
8.094
8.073
7.260
3.098
OHC
3k
1H NMR (400 MHz, CDCl3)
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.03
2.10
2.00
3.11


190.67
145.31
139.62
130.35
128.16
77.32
77.00
76.68
44.24
OHC
3k
13C NMR (100 MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



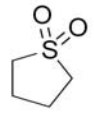
3l

^{1}H NMR (400 MHz, d^{6}-DMSO)



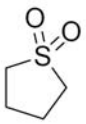
3l

^{13}C NMR (100 MHz, d^{6}-DMSO)



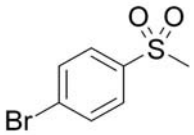
3m

^{1}H NMR (400 MHz, d^{6}-DMSO)



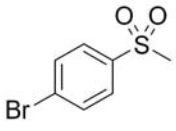
3m

^{13}C NMR (100 MHz, d^{6}-DMSO)



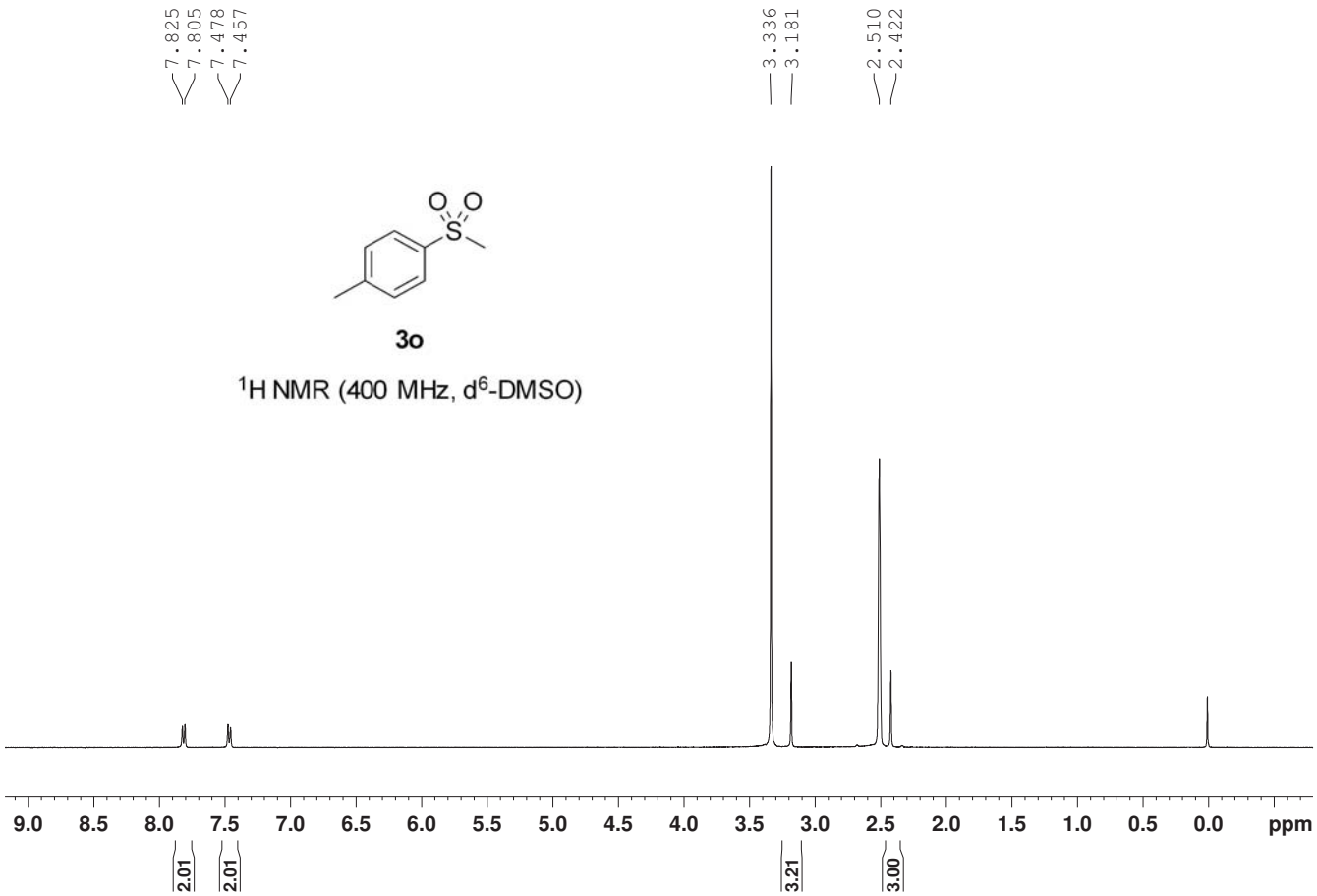
3n

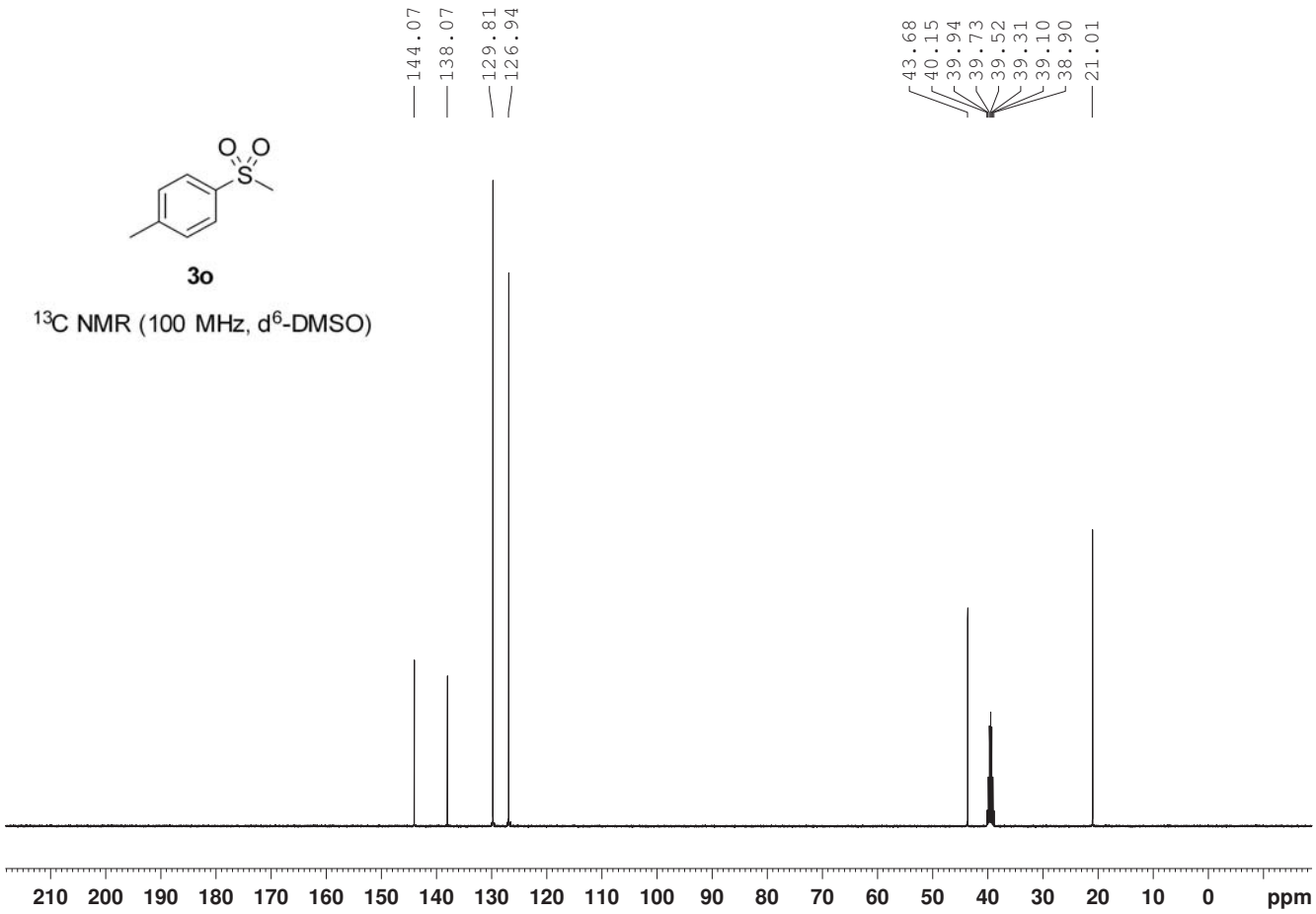
^{1}H NMR (400 MHz, d^{6}-DMSO)

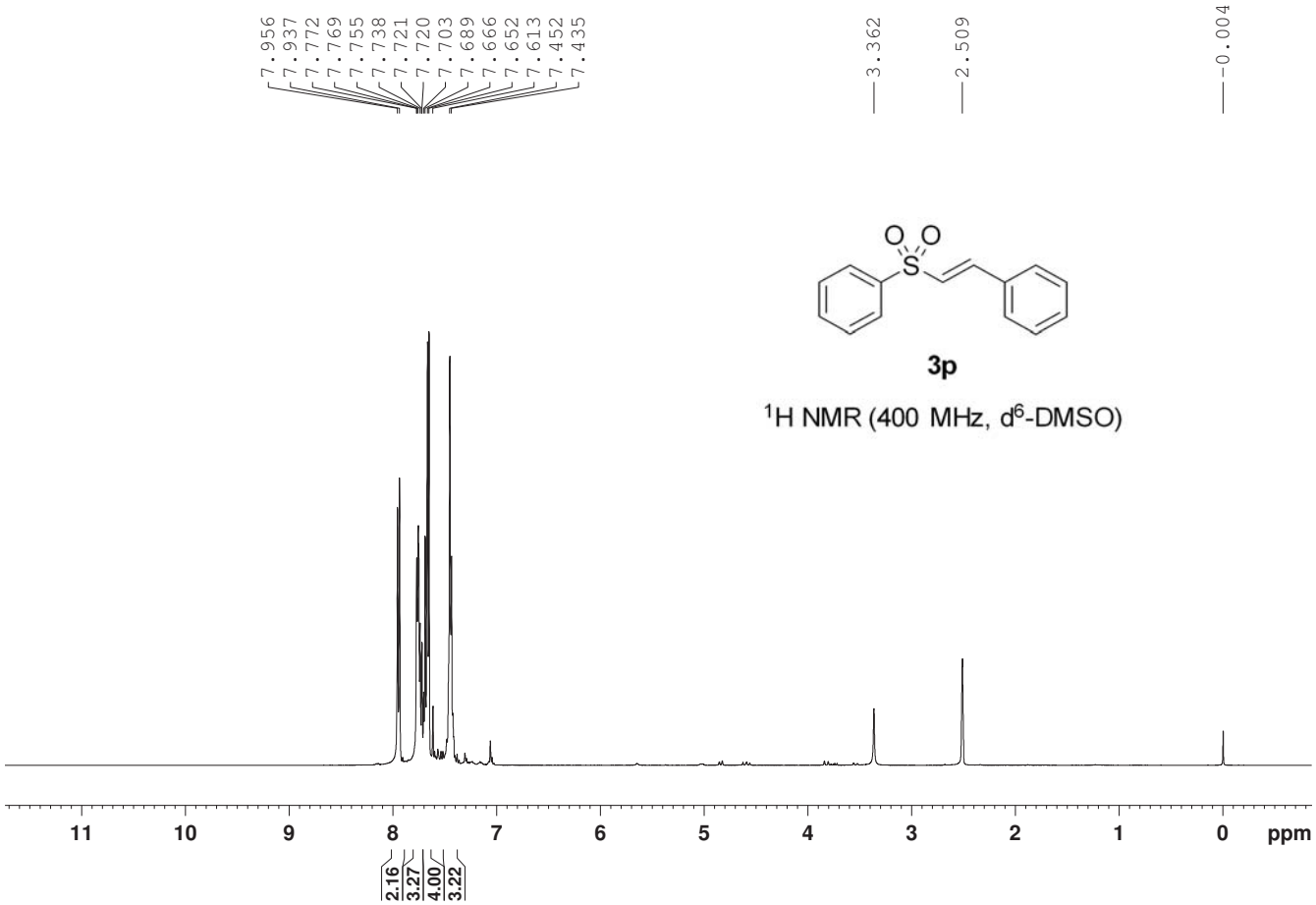


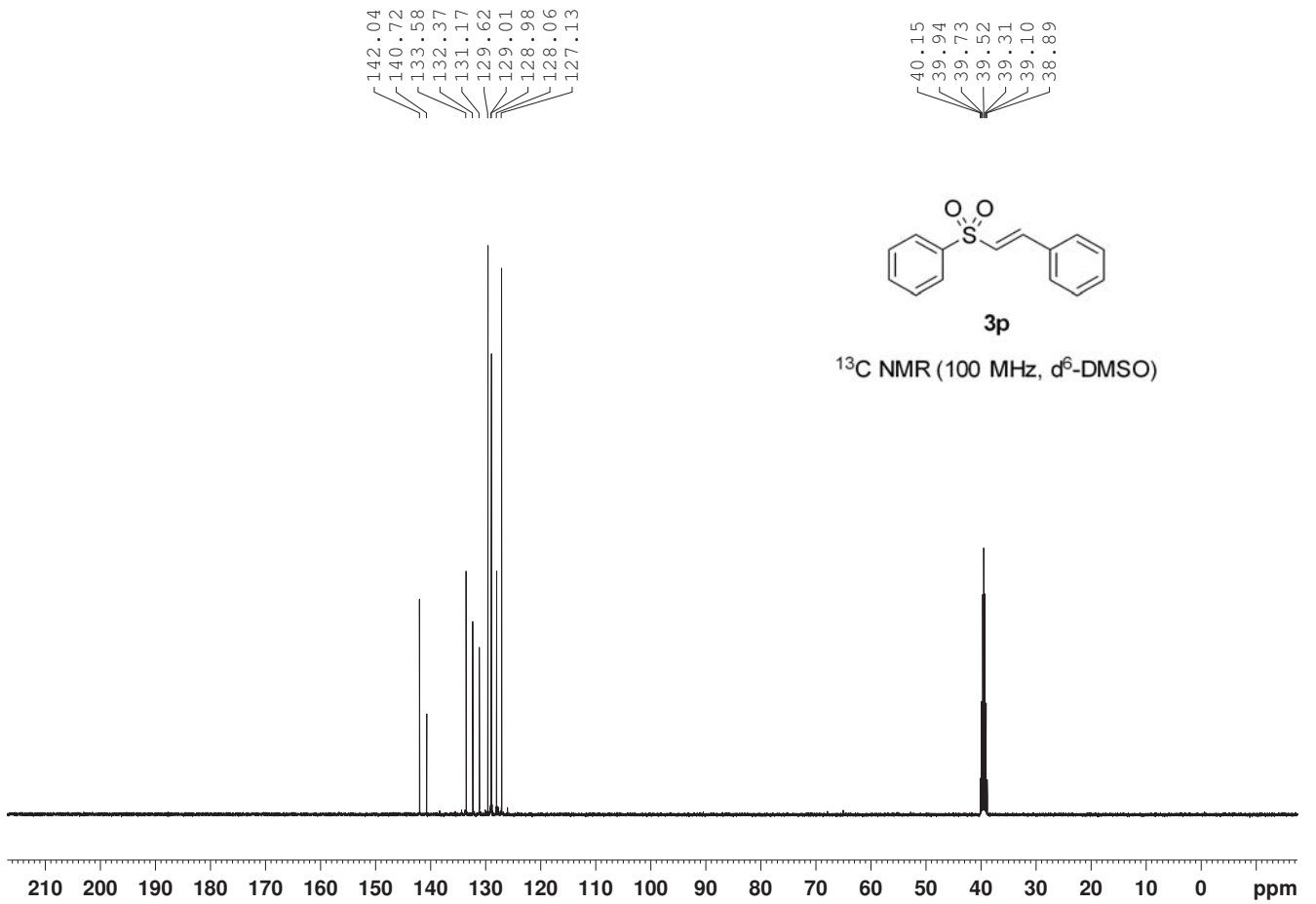
3n

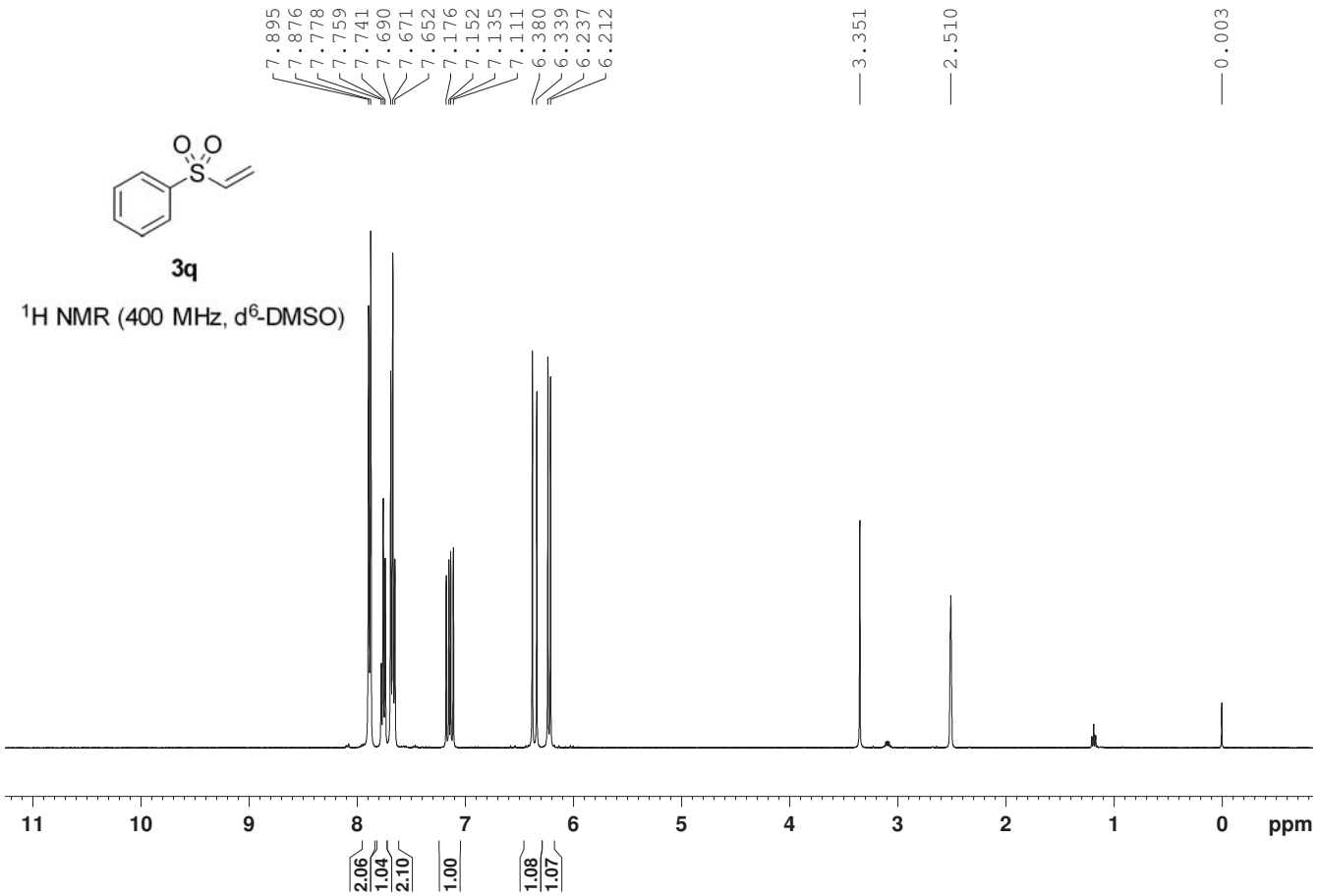
^{13}C NMR (100 MHz, d^{6}-DMSO)

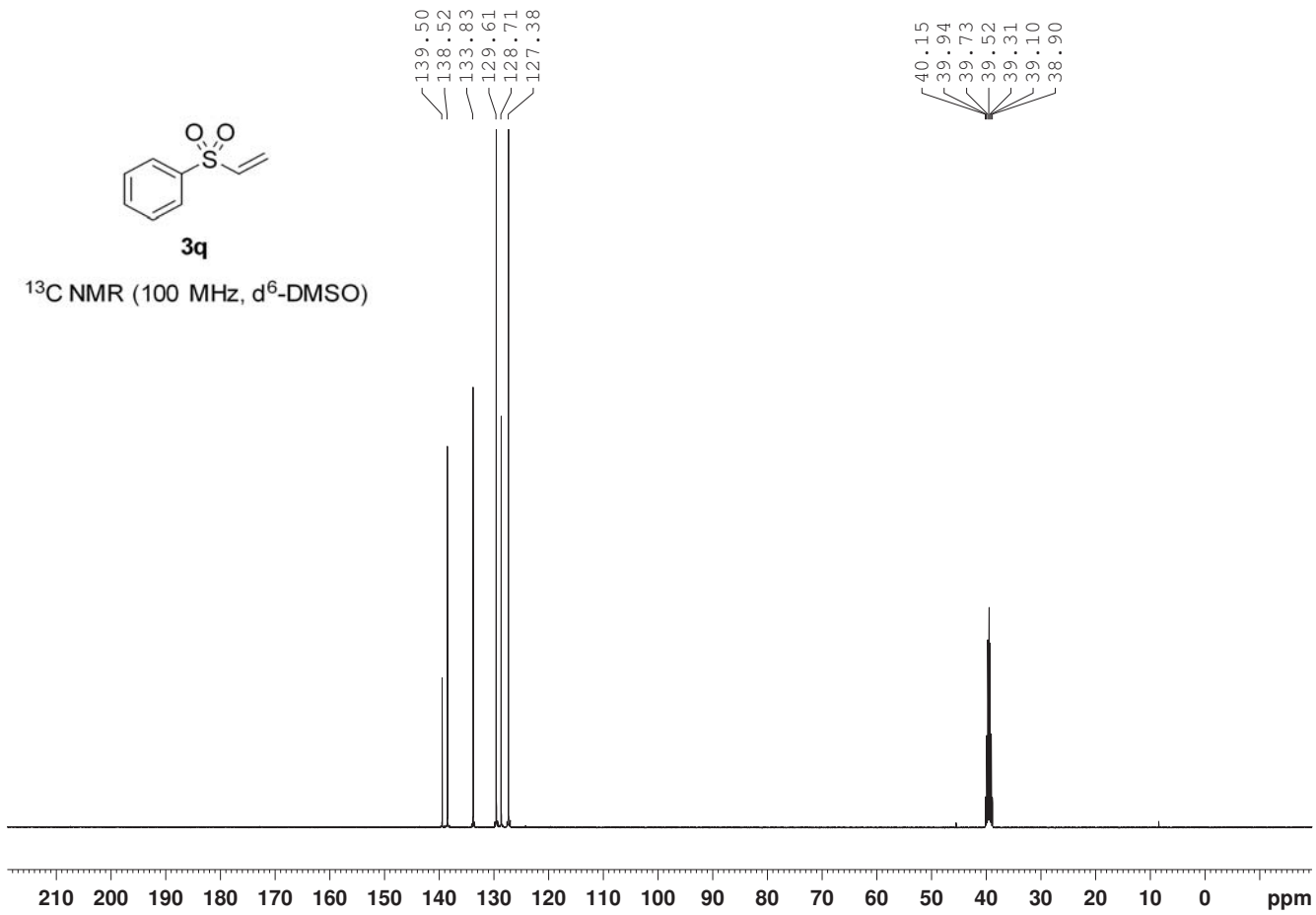

7.825
7.805
7.478
7.457
3.336
3.181
2.510
2.422
3o
1H NMR (400 MHz, d6-DMSO)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.01
2.01
3.21
3.00

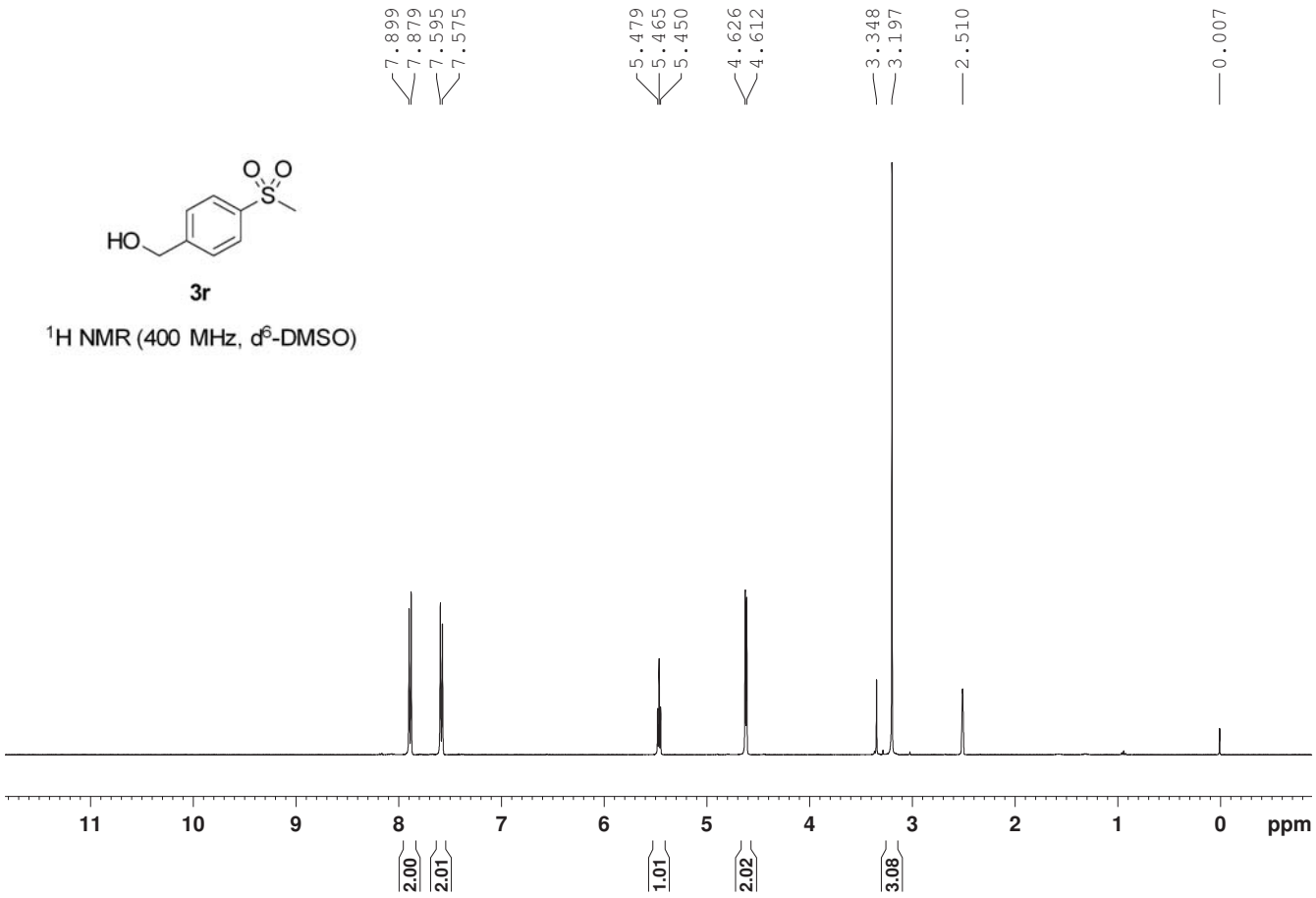

144.07
138.07
129.81
126.94
43.68
40.15
39.94
39.73
39.52
39.31
39.10
38.90
21.01
3o
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.956
7.937
7.772
7.769
7.755
7.738
7.721
7.720
7.703
7.689
7.666
7.652
7.613
7.452
7.435
3.362
2.509
0.004
3p
1H NMR (400 MHz, d6-DMSO)
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.16
3.27
4.00
3.22

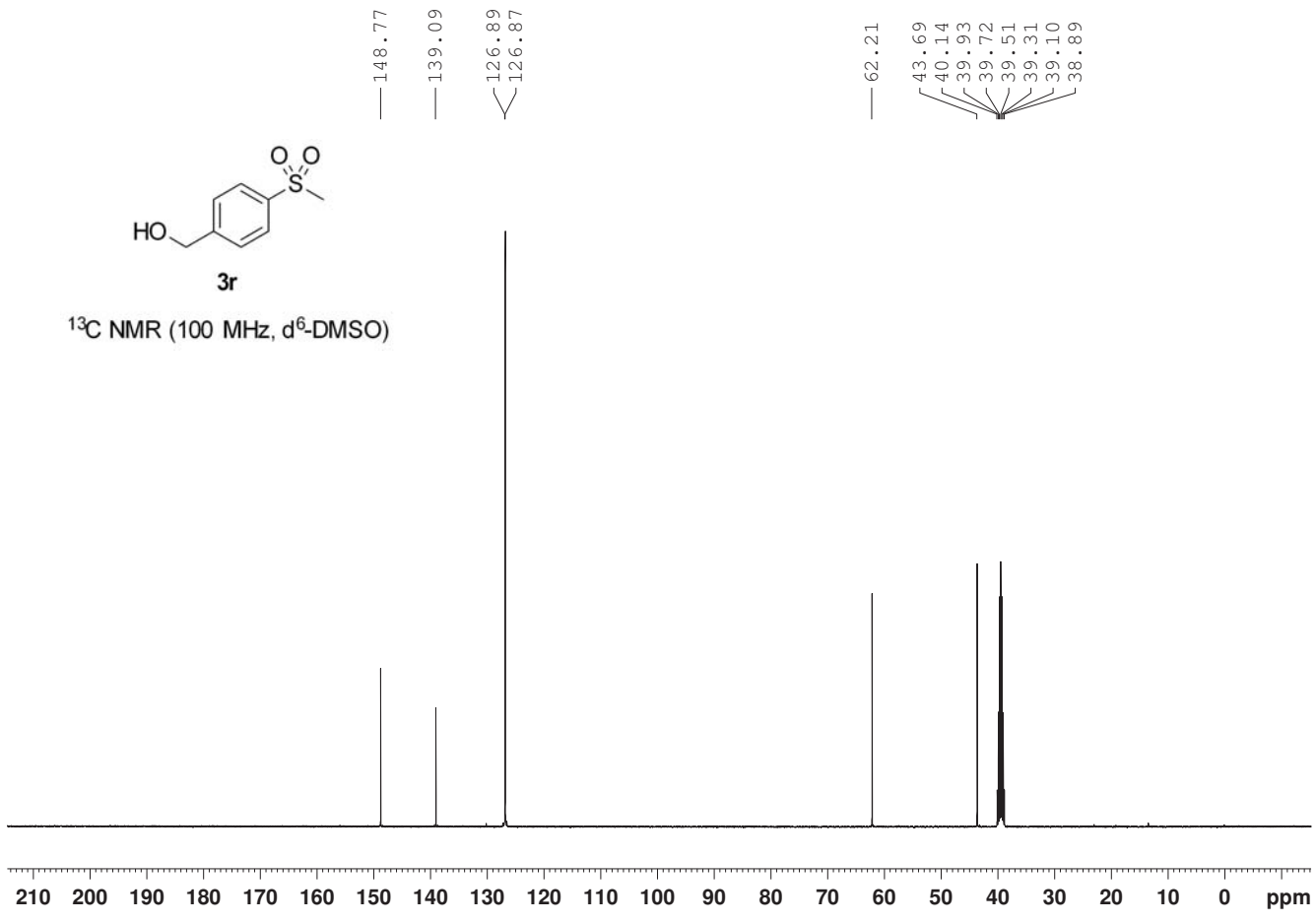

142.04
140.72
133.58
132.37
131.17
129.62
129.01
128.98
128.06
127.13
40.15
39.94
39.73
39.52
39.31
39.10
38.89
3p
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.895
7.876
7.778
7.759
7.741
7.690
7.671
7.652
7.176
7.152
7.135
7.111
6.380
6.339
6.237
6.212
3.351
2.510
0.003
3q
1H NMR (400 MHz, d6-DMSO)
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.06
1.04
2.10
1.00
1.08
1.07

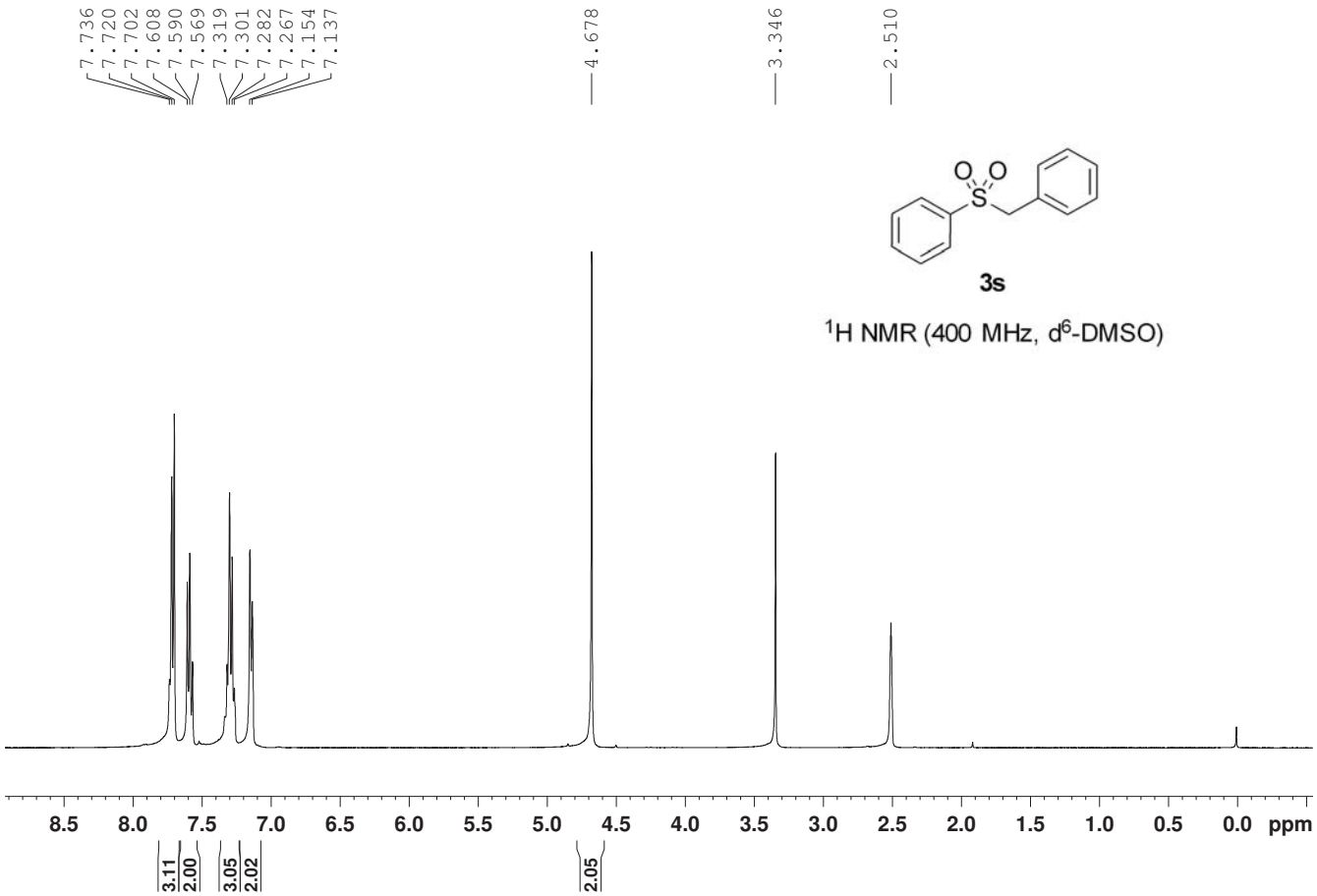

139.50
138.52
133.83
129.61
128.71
127.38
40.15
39.94
39.73
39.52
39.31
39.10
38.90
3q
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

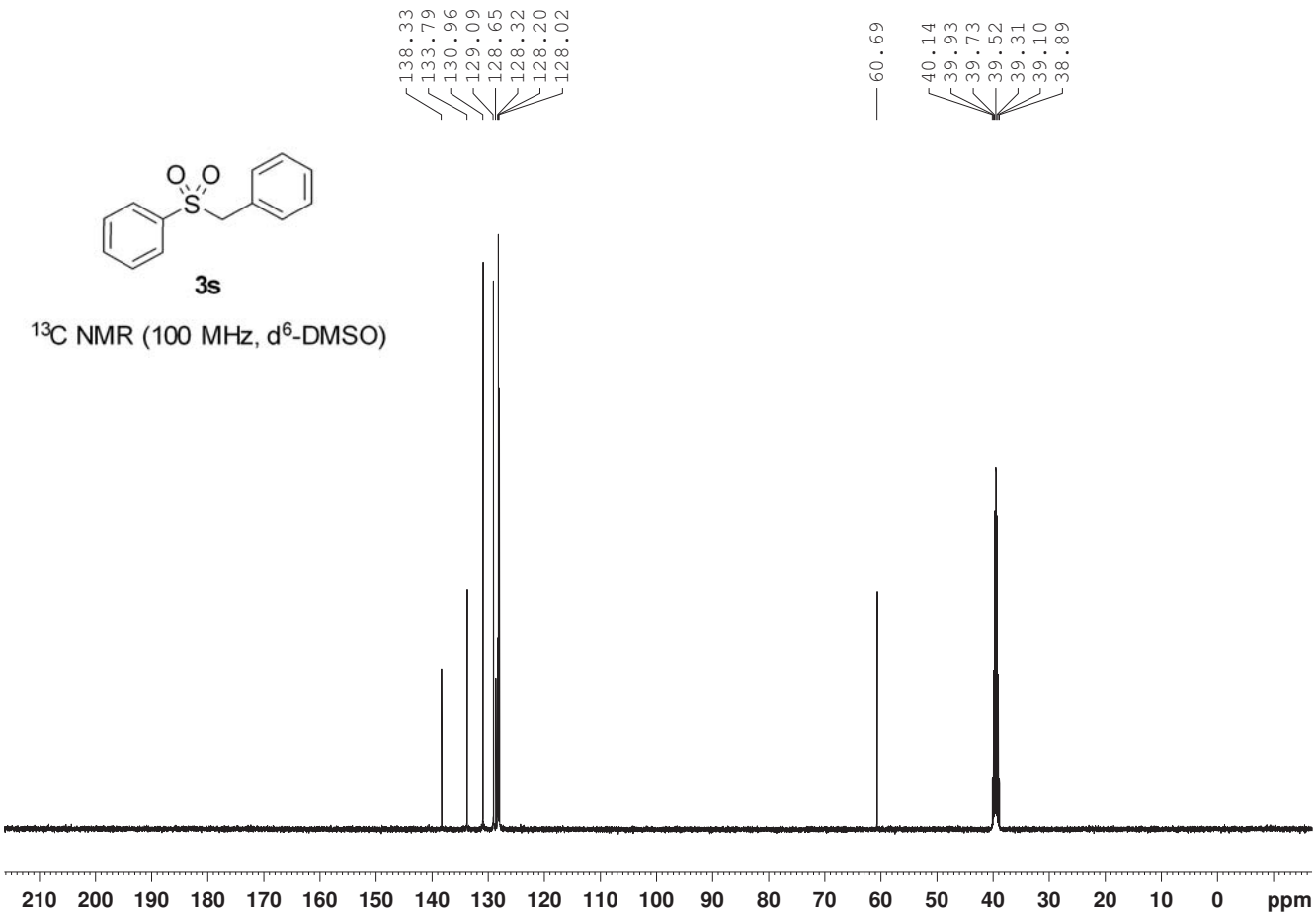


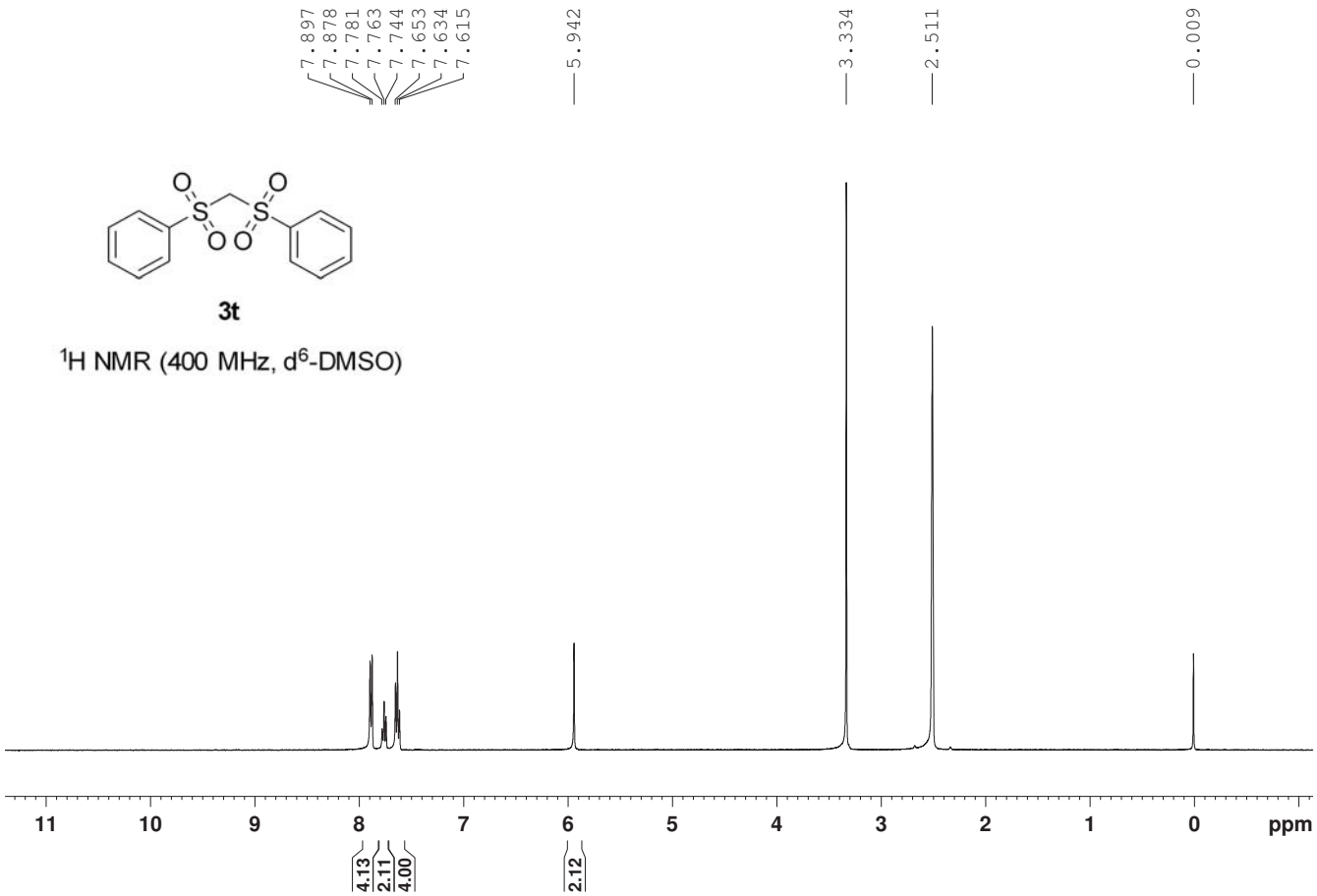
^{1}H NMR (400 MHz, d^{6}-DMSO)

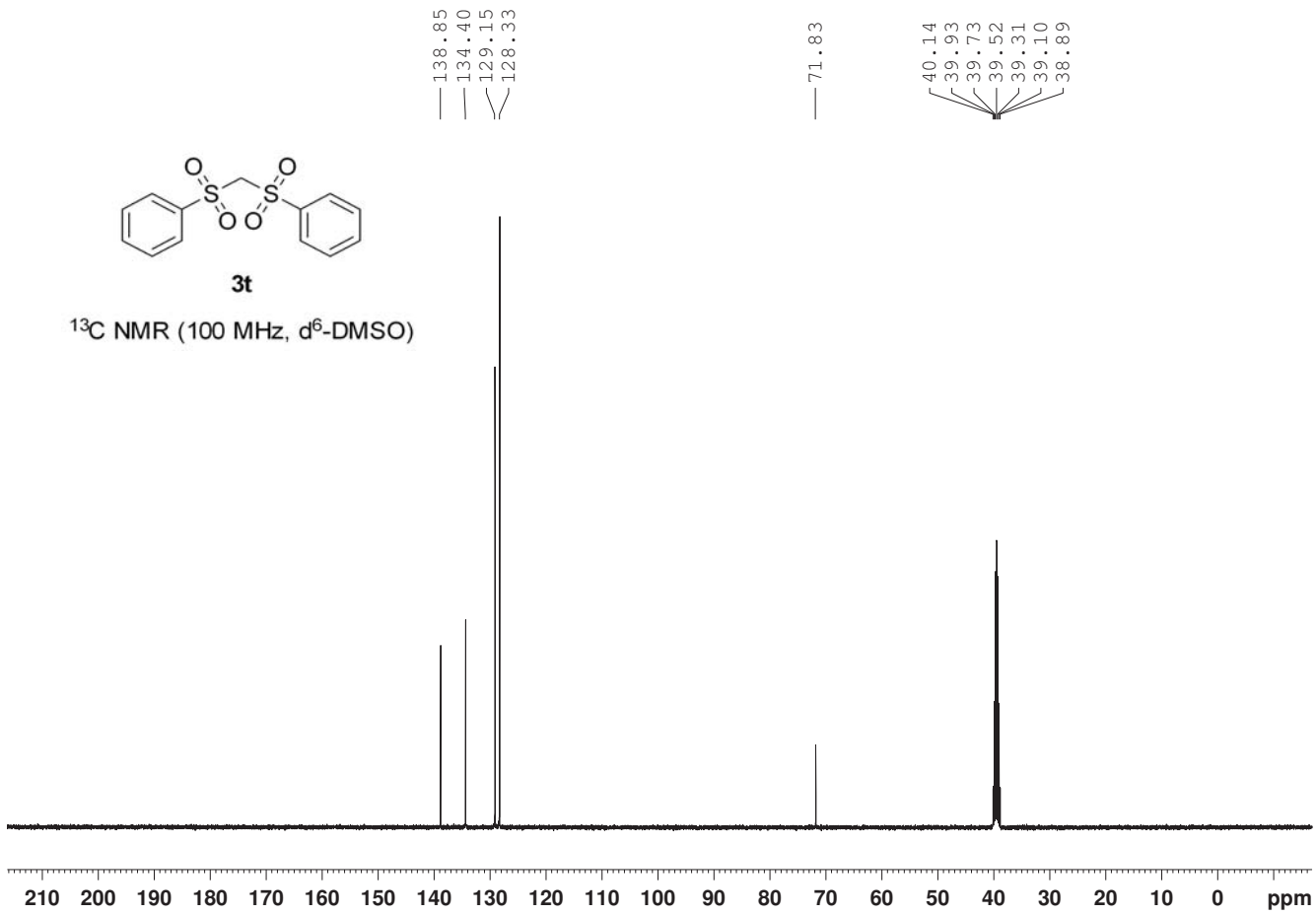


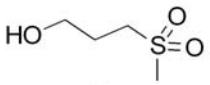
^{13}C NMR (100 MHz, d^{6}-DMSO)


7.736
7.720
7.702
7.608
7.590
7.569
7.319
7.301
7.282
7.267
7.154
7.137
4.678
3.346
2.510
3s
1H NMR (400 MHz, d6-DMSO)
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
3.11
2.00
3.05
2.02
2.05


138.33
133.79
130.96
129.09
128.65
128.32
128.20
128.02
60.69
40.14
39.93
39.73
39.52
39.31
39.10
38.89
3s
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

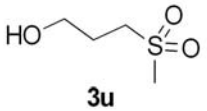

7.897
7.878
7.781
7.763
7.744
7.653
7.634
7.615
5.942
3.334
2.511
0.009
3t
1H NMR (400 MHz, d6-DMSO)
11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.13
2.11
4.00
2.12


138.85
134.40
129.15
128.33
71.83
40.14
39.93
39.73
39.52
39.31
39.10
38.89
3t
13C NMR (100 MHz, d6-DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



3u

^{1}H NMR (400 MHz, d^{6}-DMSO)



3u

^{13}C NMR (100 MHz, d^{6}-DMSO)